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13NOV03 E851660-1 D02246
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2. Patent application number *(The Patent Office will fill this part in)* — 0326396.9

3. Full name, address and postcode of the or of each applicant *(underline all surnames)* — Cyclacel Limited
12 St James's Square
London
SW1Y 4RB

Patents ADP number *(if you know it)* — 7316292004

If the applicant is a corporate body, give the country/state of its incorporation — United Kingdom

4. Title of the invention — Method

5. Name of your agent *(if you have one)* — D Young & Co

"Address for service" in the United Kingdom to which all correspondence should be sent *(including the postcode)* — 21 New Fetter Lane
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EC4A 1DA

Patents ADP number *(if you know it)* — 59006

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Continuation sheets of this form	-
Description	148
Claim(s)	9
Abstract	1
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11. I/We request the grant of a patent on the basis of this application.

Signature(s) D Young & Co. Date 12 November 2003

12. Name, daytime telephone number and e-mail address, if any, of person to contact in the United Kingdom

D Young & Co (Agents for the Applicants)
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METHOD

The present invention relates to polo-like kinases (PLKs) and small molecule inhibitors thereof. More specifically, the invention relates to a method for designing and identifying small molecule inhibitors using a homology model for PLK.

BACKGROUND TO THE INVENTION

The Polo-like kinase family consists of key cell cycle regulatory enzymes with integral roles in controlling entry into and progression through mitosis. Many tumour cells express high levels of PLK1 and are responsive to antisense oligonucleotides targeting this protein.

Initiation of mitosis requires activation of M-phase promoting factor (MPF), *i.e.* the complex between CDK1 and B-type cyclins [1]. The latter accumulate during the S and G2 phases of the cell cycle and promote the inhibitory phosphorylation of the MPF complex by WEE1, MIK1, and MYT1 kinases. At the end of the G2 phase, corresponding dephosphorylation by the dual-specificity phosphatase CDC25C triggers the activation of MPF [2]. In interphase, cyclin B localizes to the cytoplasm and becomes phosphorylated during prophase, followed by nuclear translocation. The nuclear accumulation of active MPF during prophase is thought to be important for initiating M-phase events [3]. However, nuclear MPF is kept inactive by WEE1 unless counteracted by CDC25C. The phosphatase CDC25C itself, localized to the cytoplasm during interphase, accumulates in the nucleus in prophase. The nuclear entry of both cyclin B and CDC25C are promoted through phosphorylation by PLK1 [4]. This kinase is thus an important regulator of M-phase initiation.

In humans, there exist three closely related polo-like kinases (PLKs) [5]. They contain a highly homologous N-terminal catalytic kinase domain and their C-termini contain two or three conserved regions, the polo boxes. The function of the polo boxes remains incompletely understood but polo box-dependent PLK1 activity is required for proper metaphase/anaphase transition and cytokinesis [6]. Of the three PLKs, PLK1 is the best characterized; it regulates a number of cell division cycle effects, including the onset of

mitosis, DNA-damage checkpoint activation, regulation of the anaphase promoting complex, phosphorylation of the proteasome, and centrosome duplication and maturation. Mammalian PLK2 (also known as SNK) and PLK3 (also known as PRK and FNK) were originally shown to be immediate early gene products. PLK3 kinase activity appears to peak during late S and G2 phase. It is also activated during DNA damage checkpoint activation and severe oxidative stress. PLK3 also plays an important role in the regulation of microtubule dynamics and centrosome function in the cell and deregulated PLK3 expression results in cell cycle arrest and apoptosis [7]. PLK2 is the least-well understood homologue of the three PLKs. Both PLK2 and PLK3 may have additional important post-mitotic functions [8].

The fact that human PLKs regulate some fundamental aspects of mitosis was shown by anti-PLK1 antibody microinjection of human tumour cells [9]. This treatment had no effect on DNA replication but impaired cell division. Cells were arrested in mitosis and showed abnormal distribution of condensed chromatin and monoastral microtubules nucleated from duplicated but unseparated centrosomes. By contrast, non-immortalized human cells arrested as single, mononucleated cells in G2. Moreover, when PLK1 function was blocked through adenovirus-mediated delivery of a dominant-negative gene, tumour-selective apoptosis in many tumour cell lines was observed, whereas again normal epithelial cells, although arrested in mitosis, escaped the mitotic catastrophe seen in tumour cells [10]. PLK1 activity is thus necessary for the functional maturation of centrosomes in late G2/early prophase and subsequent establishment of a bipolar spindle. Furthermore, these results suggest the presence in normal cells of a centrosome-maturation checkpoint that is sensitive to PLK1 impairment. Depletion of cellular PLK1 through the small interfering RNA (siRNA) technique also confirmed that this protein is required for multiple mitotic processes and completion of cytokinesis [11]. A potential therapeutic rationale for PLK inhibition is also suggested by work

PLK1 expression is of prognostic value for patients suffering from various types of tumours [14-16].

Although the therapeutic potential of pharmacological PLK inhibition has been appreciated [17], very little has been reported to date concerning small-molecule PLK inhibitors that may be useful as drugs. The only characterized biochemical PLK1 inhibitor is scytonemin, a symmetric indolic marine natural product [18,19]. Scytonemin inhibits phosphorylation of CDC25C by recombinant PLK1 with an IC_{50} value of about 2 μM (at an ATP concentration of 10 μM). Inhibition is apparently reversible and the mechanism with respect to ATP of mixed-competitive mode. Similar potency against other protein serine/threonine- and dual specificity cell-cycle kinases, including MYT1, CHK1, CDK1/cyclin B, and PKC, was observed. Scytonemin showed pronounced anti-proliferative effects on various human cell lines in vitro.

The present invention seeks to elucidate small molecule PLK inhibitors, and in particular, provides a method for designing and identifying such inhibitors. The invention also seeks to elucidate further information on the 3-dimensional structure of the PLK binding domain and the nature of the binding interactions between PLK and such small molecule inhibitors.

STATEMENT OF INVENTION

The present invention relates to a homology model for PLK, and the use thereof in the indentification of small molecule PLK inhibitors.

As used herein, the term "model" refers to a structural model such as a three dimensional (3D) structural model (or representation thereof) comprising PLK. Preferably, the model comprising PLK is built from all or a portion of the structure co-ordinates presented in Table 2. The homology model of the invention enables candidate compounds to be identified that bind spatially and preferentially to PLK, particularly to the active site of PLK.

Aspects of the invention are presented in the accompanying claims and are further described in the following paragraphs.

DETAILED DESCRIPTION

ASSAYS BASED ON THE PLK1 HOMOLOGY MODEL

A first aspect of the invention relates to a method of screening for a modulator of PLK, wherein the method comprises using the structure co-ordinates of Table 2

Since no experimental three-dimensional structures of PLK kinase domains are known, a PLK1 kinase domain homology model was constructed (*Example 1*) [31]. This model provides a plausible complex with the natural ligand ATP in the active site (*Figure 2*), as well as with two non-selective ATP-competitive kinase inhibitors, which were also found to inhibit PLK1, namely staurosporine [32] (IC_{50} w.r.t. PLK1 = 0.4 μM) and 4-[4-(4-methyl-2-methylamino-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol [33] (IC_{50} w.r.t. PLK1 = 4 μM) (*Figure 7*).

Of particular interest in the PLK1 kinase domain structure are Cys^{67} and Cys^{133}, both of which line the ATP binding site. Cys^{133} is located in the so-called hinge region, which is present in many kinases, and connects the N- and C-terminal lobes of the kinase domain. Its side chain projects away from the ATP-binding pocket, although its backbone NH and CO functions are probably involved in H-bonding with the purine system of ATP. The side chain of Cys^{67} on the PLK1 N-terminal lobe, on the other hand, points into the ATP-binding pocket and probably contributes directly to ATP binding *via* contacts with the ribose and/or triphosphate moieties. The position occupied by Cys^{67} in PLK1 is usually occupied by valine in other kinases and there contributes van der Waals contacts to ATP binding. A second unusual residue Phe^{133}, which is commonly leucine in other kinases, [illegible]

As discussed above, Cys^{67} of PLK1 is of particular interest, since in the modelled PLK1-ATP complex structure it is positioned closely to the ribose ring of ATP (*Figure 4a*). This situation is reminiscent of the HER-2 case as described above. More specifically, a close contact between the Cys^{67} thiol group and the 5'-O of the ribose portion of ATP is observed. A suitable adenosine-derived covalent inhibitor would thus be 5'-thioadenosine. Modelling (*Figure 4b*) of this compound into the active site of PLK1 suggests that a simple rotation of the C^{α}-C^{β} bond of Cys^{67} should accommodate this inhibitor in such a way as to bring the sulfur atoms of Cys^{67} and 5'-thioadenosine into disulfide-bonding distance without large perturbations of the bound adenine portion.

In order to test the hypothesis that Cys^{67} may indeed be involved in ATP binding by PLK1, the effect of non-specific thiol modifying agents such as thimerosal [34], N-ethylmaleimide, and iodoacetamide on PLK1 enzymatic activity was studied. All these reagents were found to inhibit CDC25C phosphorylation by PLK1 to some extent, indicating the involvement of Cys residues in enzymatic activity. The fact that such inhibition could be abolished in the presence of an excess of the reducing agent dithiothreitol, which specifically reduces disulfide bonds and competes with Cys thiol groups for thiol modifying agents [35], is consistent with this notion (*Example 6*). Adenosine derivatives were studied next (*Figure 5*). Unmodified adenosine did not inhibit PLK1 function at concentrations up to 0.2 mM, whereas 2'- and 5'-thioadenosines did. 5-Thioadenosine was about 3-fold more potent than its analogue 2'-thioadenosine, supporting the hypothesis that the 5'-OH of the ribose ring is better oriented to react with Cys^{67}. Again a lack of inhibition was observed in the presence of DTT. Kinetic analysis of PLK1 inhibition (*Example 7*) showed that with *e.g.* 5'-thioadenosine (*Figure 6*) this was dependent on ATP concentration but not competitive with ATP as would be the case for a reversible competitive ATP antagonist. The effects of the above thiol modifying reagents on a closely related serine/threonine kinase were also studied. Casein kinase II (CKII) was selected based on its sensitivity to certain inhibitors [36], *e.g.* wortmannin and LY294002 [37], which were also found to be capable of inhibiting PLK1 (IC_{50} with respect to PLK1 of < 0.1 μM and < 5 μM, respectively). No significant inhibition of CKII enzymatic activity was observed at

concentrations up to 0.2 mM with thimerosal, N-ethylmaleimide, iodoacetamide, adenosine, 2'-thioadenosine, or 5'-thioadenosine using the assay described in *Example 4*.

In summary, these results suggest that PLK-specific ATP antagonists can be developed that derive their potency and PLK selectivity from a combination of non-covalent binding to the unique ATP-binding pocket of PLK1 and covalent binding to the Cys^{67} thiol group.

Preferred embodiments of the invention will now be described.

In one preferred embodiment of the invention, the method comprises the steps of:

(a) providing at least a portion of the structure co-ordinates of Table 2;

(b) employing at least a portion of the structure co-ordinates of Table 2 to design or select or synthesise a putative modulator of PLK;

(c) contacting the putative modulator of PLK with PLK or a mutant, variant, homologue, derivative or fragment thereof, in the presence of a substrate of PLK; and

(d) determining whether said putative modulator of PLK modulates PLK.

In a preferred embodiment, at least a portion of the structure co-ordinates of Table 2 and/or the putative modulator of PLK and/or the substrate are provided on a machine-readable data storage medium comprising a data storage material encoded with machine readable data.

In a preferred embodiment, the putative modulator of PLK is selected from a library of compounds. Preferably, the library is an *in silico* library. Suitable *in silico* libraries will be

In another preferred embodiment, the putative modulator of PLK is selected from a database.

In another preferred embodiment, the putative modulator of PLK is designed *de novo*.

In yet another preferred embodiment, the putative modulator of PLK is designed from a known PLK modulator.

Preferably, the design or selection of the putative modulator of PLK is performed in conjunction with computer modelling.

In one particularly preferred embodiment, the putative modulator of PLK inhibits PLK activity.

More preferably, the PLK is PLK1.

In a further preferred embodiment, the putative modulator of PLK is useful in the prevention and/or treatment of a PLK related disorder.

Even more preferably, the PLK related disorder is a proliferative disorder.

More preferably still, the proliferative disorder is selected from cancer, leukemia, glomerulonephritis, rheumatoid arthritis, psoriasis and chronic obstructive pulmonary disorder.

A second aspect of the invention relates to an assay for a candidate compound capable of modulating PLK, said assay comprising the steps of:

(a) contacting said candidate compound with PLK;

(b) detecting whether said candidate compound forms associations with one or more amino acid residues corresponding to PLK amino acid residues L59, G60, C67, A80, K82, L130, C133, R135, F183 and D194.

In one preferred embodiment, said candidate compound is selected by performing rational drug design with a 3-dimensional model of PLK in conjunction with computer modelling.

In an even more preferred embodiment, the assay comprises detecting whether said candidate compound forms an association with the amino acid residue corresponding to PLK amino acid residue C67.

A third aspect of the invention relates to the use of a compound selected from the following:

(i) 5'-thioadenosine, or a derivative thereof;

(ii) staurosporine, or a derivative thereof; and

(iii) 4-[4-(4-methyl-2-methylaminothiazol-5-yl)-pyrimidin-2-ylamino]-phenol; 4-[4-(2,4-dimethyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol or 4-[4-(2-amino-4-methyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol;

or a pharmaceutically acceptable salt thereof, in an assay for identifying candidate compounds capable of modulating PLK.

Preferably, the assay is a competitive binding assay.

More preferably, the assay comprises contacting a candidate compound with PLK in the presence of a compound selected from:

(i) 5'-thioadenosine, or a derivative thereof;

(ii) staurosporine, or a derivative thereof; and

(iii) 4-[4-(4-methyl-2-methylaminothiazol-5-yl)-pyrimidin-2-ylamino]-phenol, 4-[4-(2,4-dimethyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol or 4-[4-(2-amino-4-methyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol;

or a pharmaceutically acceptable salt thereof, and detecting any change in the

(a) a computer-readable data storage medium comprising a data storage material encoded with computer-readable data, wherein said data comprises the structure co-ordinates of Table 2;

(b) a working memory for storing instructions for processing said computer-readable data;

(c) a central-processing unit coupled to said working memory and to said computer-readable data storage medium for processing said computer-machine readable data into said three-dimensional representation; and

(d) a display coupled to said central-processing unit for displaying said three-dimensional representation.

Another aspect of the invention relates to a machine-readable data storage medium comprising a data storage material encoded with machine readable data, wherein the data is defined by at least a portion of the structure co-ordinates of Table 2.

A further aspect of the invention relates to the use of the above-described computer or machine readable data storage medium to predict the structure and/or function of potential modulators of PLK.

Another aspect relates to the use of at least a portion of the structure co-ordinates of Table 2 to screen for modulators of PLK.

A further aspect relates to the use of at least a portion of the structure co-ordinates of Table 2 to solve the structure of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of PLK.

Preferably, the structure of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of PLK is solved using molecular replacement.

Yet another aspect of the invention relates to the use of at least a portion of the structure co-ordinates of Table 2 in molecular design techniques to design, select and synthesise modulators of PLK.

A further aspect of the invention relates to the use of at least a portion of the structure co-ordinates of Table 2 in the development of compounds that can isomerise to reaction intermediates in the chemical reaction of a substrate or other compound that binds to PLK.

Another aspect of the invention relates to the use of at least a portion of the structure co-ordinates of Table 2 to screen small molecule databases for chemical entities or compounds that modulate PLK.

PLK MODULATORS

A further aspect of the invention relates to a PLK modulator identified by the above-described method, or a candidate compound identified by the above-described assay.

Preferably, the PLK modulator or candidate compound of the invention inhibits PLK activity.

More preferably, the PLK modulator or candidate compound of the invention is capable of forming a covalent bond with the amino acid residue corresponding to PLK amino acid residue C67.

More preferably still, the PLK modulator or candidate compound of the invention is capable of forming a disulfide bond with the thiol group of the amino acid residue corresponding to PLK amino acid residue C67.

The present invention permits the use of molecular design techniques to design, select and synthesise chemical entities and compounds, including PLK modulating compounds, capable of binding to PLK, in whole or in part.

By way of example, the structure co-ordinates of Table 2 may be used to design compounds that bind to PLK and may alter the physical properties of the compounds (eg. solubility) or PLK itself. This invention may be used to design compounds that act as modulators, such as competitive inhibitors - of PLK by binding to all or a portion of the active site of PLK. Compounds may also be designed that act as non-competitive inhibitors of PLK. These non-competitive inhibitors may bind to all or a portion of PLK already bound to its substrate and may be more potent and specific than known PLK inhibitors that compete only for the PLK active site. Similarly, non-competitive inhibitors that bind to and inhibit PLK whether or not it is bound to another chemical entity may be designed using the structure co-ordinates of PLK described herein.

The present invention may also allow the development of compounds that can isomerise to reaction intermediates in the chemical reaction of a substrate or other compound that binds to PLK. Thus, the time-dependent analysis of structural changes in PLK during its interaction with other molecules may be performed. The reaction intermediates of PLK may also be deduced from the reaction product in co-complex with PLK. Such information is especially useful to design improved analogues of known PLK modulators or to design new PLK modulators based on the reaction intermediates of the PLK enzyme and PLK-modulator complex. This may provide a new route for designing PLK modulators with high specificity and stability. Preferably, this provides a new route for designing PLK modulators with high specificity, high stability and low toxicity.

Small molecule databases or candidate compounds may be screened for chemical entities or compounds that can bind in whole, or in part, to PLK. Thus, in a preferred embodiment, the putative PLK modulator is from a library of compounds or a database. In this screening, the quality of fit of such entities or compounds to the binding site

may be judged by various methods – such as shape complementarity or estimated interaction energy (Meng, E. C. *et al., J. Comp. Chem.*, 13, pp. 505-524 (1992)).

The structure co-ordinates of Table 2, or portions thereof, may also be useful in solving the structure of crystal forms of PLK. They may also be used to solve the structure of PLK mutants, PLK variants, PLK homologues, PLK derivatives, PLK fragments and PLK complexes.

Preferably, the structure co-ordinates of Table 2 may be used to solve the structure of the crystalline form of proteins having significant amino acid sequence homology to any functional domain of PLK. By way of example, molecular replacement may be used. In this method, the unknown crystal structure, whether it is a crystal form of PLK, a PLK mutant, a PLK variant, a PLK homologue (eg. another protein with significant amino acid sequence homology to any functional domain of PLK), a PLK derivative, a PLK fragment or a PLK co-complex may be determined using the PLK structure co-ordinates of the present invention. This method will provide a more accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information *ab initio*.

In a preferred embodiment of the present invention, the PLK crystal of unknown structure further comprises an entity bound to the PLK protein or a portion thereof, for example, an entity that is an inhibitor of PLK.

The crystal structures of such complexes may be solved by molecular replacement or in combination with MAD (Multiwavelength Anomalous Dispersion) and/or MIRAS (Multiple Isomorphous Replacement with Anomalous Scattering) procedures - and compared with that of wild-type PLK. Potential sites for modification within the

The structures and complexes of PLK may be refined using computer software - such as X-PLOR (Meth. Enzymol., vol. 114 & 115, H. W. Wyckoff et al., eds., Academic Press (1985)), MLPHARE (Collaborative computational project Number 4. The CCP4 Suite: Programs for Protein Crystallography (1994) Acta Crystallogr. D 50, 760-763) and SHARP [De La Fortelle, E. & Bricogne, G. Maximum-likelihood heavy-atom parameters refinement in the MIR and MAD methods (1997) Methods Enzymol. 276, 472-494). Preferably, the complexes are refined using the program CNS (Brünger *et al.* (1998) *Acta Crystallogr.* D 54, 905-921). During the final stages of refinement water molecules, ions and inhibitor molecules may be inserted in the structure. This information may thus be used to optimise known classes of PLK modulators, eg. PLK inhibitors, and more importantly, to design and synthesise novel classes of PLK modulators.

The overall figure of merit may be improved by iterative solvent flattening, phase combination and phase extension with the program SOLOMON [Abrahams, J. P. & Leslie, A. G. W. Methods used in structure determination of bovine mitochondrial F1 ATPase. (1996) Acta Crystallogr. D 52, 110-119].

The structure co-ordinates of the homology model of the present invention may also facilitate the identification of related proteins or enzymes analogous to PLK in function, structure or both, thereby further leading to novel therapeutic modes for treating or preventing PLK related diseases.

The design of compounds that bind to or modulate PLK according to the present invention generally involves consideration of two factors. Firstly, the compound must be capable of physically and structurally associating with PLK. Non-covalent molecular interactions important in the association of PLK with its substrate may include hydrogen bonding, van der Waals and hydrophobic interactions. Secondly, the compound must be able to assume a conformation that allows it to associate with PLK. Although certain portions of the compound may not directly participate in the association with PLK, those portions may still influence the overall conformation of the molecule. This may have a significant impact on potency. Such conformational

requirements include the overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of a binding site of PLK, or the spacing between functional groups of a compound comprising several chemical entities that directly interact with PLK.

The potential modulating or binding effect of a chemical compound on PLK may be analysed prior to its actual synthesis and testing by the use of computer modelling techniques. If the theoretical structure of the given compound suggests insufficient interaction and association with PLK, then synthesis and testing of the compound may be obviated. However, if computer modelling indicates a strong interaction, the molecule may be synthesised and tested for its ability to bind to PLK and modulate (eg. inhibit) using the fluorescent substrate assay of Thornberry *et al.* (2000) *Methods Enzymol.* 322, pp 100-110. In this manner, synthesis of inactive compounds may be avoided.

A modulating or other binding compound of PLK may be computationally evaluated and designed by means of a series of steps in which chemical entities or candidate compounds are screened and selected for their ability to associate with PLK.

A person skilled in the art may use one of several methods to screen chemical entities or candidate compounds for their ability to associate with PLK and more particularly with the individual binding sites of PLK. This process may begin by visual inspection of, for example, the active site on the computer screen based on the PLK co-ordinates of the present invention. Selected chemical entities or candidate compounds may then be positioned in a variety of orientations, or docked, with PLK. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimisation and molecular dynamics with standard molecular mechanics force fields -

(Goodford (1985) J. Med. Chem., 28, pp. 849-857) and AUTODOCK (Goodsell and Olsen (1990), Proteins: Structure. Function, and Genetics, 8, pp. 195-202.

Once suitable chemical entities or candidate compounds have been selected, they may be assembled into a single compound, such as a PLK modulator. Assembly may proceed by visual inspection of the relationship of the chemical entities or candidate compounds in relation to the structure co-ordinates of PLK. This may be followed by manual model building using software - such as Quanta, Sybyl, O, HOOK or CAVEAT [Jones, T. A., Zou, J. Y., Cowan, S. W. & Kjeldgaard, M. Improved methods for building protein models in electron density maps and the location of errors in these models (1991) Acta Crystallogr. A 47, 110-119].

Refinement of the model may be carried out using the program CNS [Brünger, A. T. et al. Crystallography & NMR System: A new software suite for macromolecular structure determination. (1998) Acta Crystallogr. D 54, 905-921].

Various programs may be used by a skilled person to connect the individual chemical entities or candidate compounds, such as 3D Database systems (Martin (1992) *J. Med. Chem.*, 35, pp. 2145-2154) and CAVEAT (Bartlett *et al.* (1989) *Royal Chem. Soc.* 78, pp. 182-196).

Rather than build a PLK inhibitor one chemical entity at a time, modulating or other PLK binding compounds may be designed as a whole or *de novo* using either an empty binding site or optionally including some portion(s) of a known inhibitor(s). Such compounds may be designed using programs that may include but are not limited to LEGEND (Nishibata and Itai (1991) Tetrahedron, 47, p. 8985) and LUDI (Bohm (1992) *J. Comp. Aid. Molec. Design*, 6, pp. 61-78).

Other molecular modelling techniques may also be employed in accordance with this invention – such as those described by Cohen et al., J. Med. Chem., 33, pp. 883-894 (1990); Navia and Murcko (1992) Current Opinions in Structural Biology, 2, pp. 202-210 (1992).

Once a compound has been designed or selected by the above methods, the efficiency with which that compound may bind to PLK may be computationally evaluated. Specific computer software may be used to evaluate the efficiency of binding (eg. to evaluate compound deformation energy and electrostatic interaction), such as QUANTA/CHARMM (Accelrys Inc., USA) and Insight II/Discover (Biosym Technologies Inc., San Diego, Calif., USA). These programs may be implemented, for instance, using a suitable workstation. Other hardware systems and software packages will be known to those persons skilled in the art.

Once a PLK-modulating compound has been selected or designed, as described above, substitutions may be made (eg. in atoms or side groups) to improve or modify the binding properties. The substitutions may be conservative ie. the replacement group may have approximately the same size, shape, hydrophobicity and charge as the original group. Such substituted chemical compounds may then be analysed for efficiency of binding to PLK by the same computer methods described above.

Candidate compounds and modulators of PLK etc. which are identified using the methods of the present invention may be screened in assays. Screening can be, for example *in vitro*, in cell culture, and/or *in vivo*. Biological screening assays preferably centre on activity-based response models, binding assays (which measure how well a compound binds), and bacterial, yeast and animal cell lines (which measure the biological effect of a compound in a cell). The assays can be automated for high capacity-high throughput screening (HTS) in which large numbers of compounds can be tested to identify compounds with the desired activity.

Current screening technologies are described in Handbook of Drug Screening, edited by Ramakrishna Seethala, Prabhavathi B. Fernandes. New York, NY, Marcel Dekker, [illegible]

The term "PLK modulator" may refer to a single entity or a combination of entities.

The PLK modulator may be an antagonist or an agonist of PLK.

As used herein, the term "agonist" means any entity, which is capable of interacting (eg. binding) with PLK and which is capable of increasing a proportion of the PLK that is in an active form, resulting in an increased biological response.

As used herein, the term "antagonist" means any entity, which is capable of interacting (eg. binding) with PLK and which is capable of decreasing (eg. inhibiting) a proportion of the PLK that is in an active form, resulting in a decreased biological response.

Preferably, the PLK modulators of the present invention are antagonists of PLK.

The modulator of PLK may be an organic compound or other chemical. The modulator of PLK may be a compound, which is obtainable from or produced by any suitable source, whether natural or artificial. The modulator of PLK may be an amino acid molecule, a polypeptide, or a chemical derivative thereof, or a combination thereof. The modulator of PLK may even be a polynucleotide molecule, which may be a sense or an anti-sense molecule. The modulator of PLK may even be an antibody.

The modulator of PLK may be designed or obtained from a library of compounds, which may comprise peptides, as well as other compounds, such as small organic molecules.

By way of example, the modulator of PLK may be a natural substance, a biological macromolecule, or an extract made from biological materials such as bacteria, fungi, or animal (particularly mammalian) cells or tissues, an organic or an inorganic molecule, a synthetic agent, a semi-synthetic agent, a structural or functional mimetic, a peptide, a peptidomimetic, a derivatised agent, a peptide cleaved from a whole protein, or a peptide synthesised synthetically (such as, by way of example, either using a peptide synthesiser or by recombinant techniques or combinations thereof, a recombinant agent,

an antibody, a natural or a non-natural agent, a fusion protein or equivalent thereof and mutants, derivatives or combinations thereof).

Typically, the modulator of PLK will be an organic compound. Typically, the organic compounds will comprise two or more hydrocarbyl groups. Here, the term "hydrocarbyl group" means a group comprising at least C and H and may optionally comprise one or more other suitable substituents. Examples of such substituents may include halo-, alkoxy-, nitro-, an alkyl group, a cyclic group etc. In addition to the possibility of the substituents being a cyclic group, a combination of substituents may form a cyclic group. If the hydrocarbyl group comprises more than one C then those carbons need not necessarily be linked to each other. For example, at least two of the carbons may be linked *via* a suitable element or group. Thus, the hydrocarbyl group may contain hetero atoms. Suitable hetero atoms will be apparent to those skilled in the art and include, for instance, sulphur, nitrogen and oxygen. For some applications, preferably the modulator of PLK comprises at least one cyclic group. The cyclic group may be a polycyclic group, such as a non-fused polycyclic group. For some applications, the modulator of PLK comprises at least the one of said cyclic groups linked to another hydrocarbyl group.

The modulator of PLK may contain halo groups, for example, fluoro, chloro, bromo or iodo groups, or one or more of alkyl, alkoxy, alkenyl, alkylene and alkenylene groups, each of which may be branched or unbranched.

The modulator of PLK may be a structurally novel modulator of PLK, or may be an analogue of a known modulator of PLK.

Preferably, the PLK modulators have improved properties over those previously

The modulator of PLK may be used in combination with one or more other pharmaceutically active agents. If combinations of active agents are administered, then they may be administered simultaneously, separately or sequentially.

CANDIDATE COMPOUNDS

As used herein, the term "candidate compound" includes, but is not limited to, a compound which may be obtainable from or produced by any suitable source, whether natural or not.

The candidate compound may be designed or obtained from a library of compounds, which may comprise peptides, as well as other compounds, such as small organic molecules and particularly new lead compounds. By way of example, the candidate compound may be a natural substance, a biological macromolecule, or an extract made from biological materials - such as bacteria, fungi, or animal (particularly mammalian) cells or tissues, an organic or an inorganic molecule, a synthetic candidate compound, a semi-synthetic candidate compound, a structural or functional mimetic, a peptide, a peptidomimetic, a derivatised candidate compound, a peptide cleaved from a whole protein, or a peptide synthesised synthetically, for example, either using a peptide synthesiser or by recombinant techniques or combinations thereof, a recombinant candidate compound, a natural or a non-natural candidate compound, a fusion protein or equivalent thereof and mutants, derivatives or combinations thereof. The candidate compound may even be a compound that is a modulator of PLK, such as a known inhibitor of PLK, that has been modified in some way eg. by recombinant DNA techniques or chemical synthesis techniques.

Typically, the candidate compound will be prepared by recombinant DNA techniques and/or chemical synthesis techniques.

Once a candidate compound capable of interacting PLK has been identified, further steps may be carried out to select and/or to modify the candidate compounds and/or to modify existing compounds, such that they are able to modulate PLK.

In one aspect, the modulator of PLK may act as a model (for example, a template) for the development of other compounds.

A further aspect relates to the use of candidate compounds or PLK modulators identified by the assays and methods of the invention in one or more model systems, for example, in a biological model, a disease model, or a model for PLK inhibition. Such models may be used for research purposes and for elucidating further details of the biological, physicochemical, pharmacological and/or pharmacokinetic activity of a particular candidate compound. By way of example, the candidate compounds or PLK modulators of the present invention may be used in biological models or systems in which the cell cycle is known to be of particular significance, e.g. in models relating to cell fertilization, especially in animals.

MIMETIC

As used herein, the term "mimetic" relates to any chemical which includes, but is not limited to, a peptide, polypeptide, antibody or other organic chemical which has the same qualitative activity or effect as a known compound. That is, the mimetic is a functional equivalent of a known compound.

CHEMICAL SYNTHESIS METHODS

Preferably, the modulator of PLK of the present invention may be prepared by chemical synthesis techniques.

It will be apparent to those skilled in the art that sensitive functional groups may need to be protected and deprotected during synthesis of a compound of the invention. This may be achieved by conventional techniques, for example as described in "Protective Groups in Organic Synthesis" by T W Greene and P G M Wuts, John Wiley and Sons Inc. (1991),

possible during e.g. a guanylation step. It should be possible to circumvent potential problems such as this by choice of reaction sequence, conditions, reagents, protection/deprotection regimes, etc. as is well-known in the art.

The compounds and salts may be separated and purified by conventional methods.

Separation of diastereomers may be achieved by conventional techniques, e.g. by fractional crystallisation, chromatography or H.P.L.C. of a stereoisomeric mixture of a compounds or suitable salts or derivatives thereof. An individual enantiomer of a compound may also be prepared from a corresponding optically pure intermediate or by resolution, such as by H.P.L.C. of the corresponding racemate using a suitable chiral support or by fractional crystallisation of the diastereomeric salts formed by reaction of the corresponding racemate with a suitably optically active acid or base.

PLK, modulators of PLK or variants, homologues, derivatives, fragments or mimetics thereof may be produced using chemical methods to synthesise the PLK or the modulator of PLK in whole or in part. For example, a PLK peptide or a modulator of PLK that is a peptide can be synthesised by solid phase techniques, cleaved from the resin, and purified by preparative high performance liquid chromatography (e.g., Creighton (1983) Proteins Structures And Molecular Principles, WH Freeman and Co, New York NY). The composition of the synthetic peptides may be confirmed by amino acid analysis or sequencing (e.g., the Edman degradation procedure; Creighton, *supra*).

Synthesis of peptides (or variants, homologues, derivatives, fragments or mimetics thereof) may be performed using various solid-phase techniques (Roberge JY *et al* (1995) Science 269: 202-204) and automated synthesis may be achieved, for example, using the ABI 43 1 A Peptide Synthesizer (Perkin Elmer) in accordance with the instructions provided by the manufacturer. Additionally, the amino acid sequences comprising the modulator of PLK, may be altered during direct synthesis and/or combined using chemical methods with a sequence from other subunits, or any part thereof, to produce a variant modulator of PLK.

CHEMICAL MODIFICATION

In one embodiment, the modulator of PLK may be a chemically modified modulator of PLK. The chemical modification of a modulator of PLK may either enhance or reduce interactions between the modulator of PLK and the target, such as hydrogen bonding interactions, charge interactions, hydrophobic interactions, van der Waals interactions or dipole interactions.

PROCESS

Another aspect of the invention relates to a process comprising the steps of:

(a) performing the method according to the invention, or an assay according to the invention;

(b) identifying one or more modulators of PLK; and

(c) preparing a quantity of said one or more PLK modulators.

A further aspect of the invention relates to a process comprising the steps of:

(a) performing the method according to the invention, or an assay according to the invention;

(b) identifying one or more PLK modulators; and

(c) preparing a pharmaceutical composition comprising said one or more identified PLK modulators.

A further aspect relates to a process comprising the steps of:

(a) performing the method according to the invention, or an assay according to the invention;

(b) identifying one or more PLK modulators;

(c) modifying said one or more PLK modulators; and

(d) optionally preparing a pharmaceutical composition comprising said one or more

acceptable carrier, diluent, excipient or adjuvant or any combination thereof. Even though the PLK modulators or candidate compounds (including their pharmaceutically acceptable salts, esters and pharmaceutically acceptable solvates) can be administered alone, they will generally be administered in admixture with a pharmaceutical carrier, excipient or diluent, particularly for human therapy. The pharmaceutical compositions may be for human or animal usage in human and veterinary medicine.

Examples of such suitable excipients for the various different forms of pharmaceutical compositions described herein may be found in the "Handbook of Pharmaceutical Excipients, 2nd Edition, (1994), Edited by A Wade and PJ Weller.

Acceptable carriers or diluents for therapeutic use are well known in the pharmaceutical art, and are described, for example, in Remington's Pharmaceutical Sciences, Mack Publishing Co. (A. R. Gennaro edit. 1985).

Examples of suitable carriers include lactose, starch, glucose, methyl cellulose, magnesium stearate, mannitol, sorbitol and the like. Examples of suitable diluents include ethanol, glycerol and water.

The choice of pharmaceutical carrier, excipient or diluent can be selected with regard to the intended route of administration and standard pharmaceutical practice. The pharmaceutical compositions may comprise as, or in addition to, the carrier, excipient or diluent any suitable binder(s), lubricant(s), suspending agent(s), coating agent(s), solubilising agent(s).

Examples of suitable binders include starch, gelatin, natural sugars such as glucose, anhydrous lactose, free-flow lactose, beta-lactose, corn sweeteners, natural and synthetic gums, such as acacia, tragacanth or sodium alginate, carboxymethyl cellulose and polyethylene glycol.

Examples of suitable lubricants include sodium oleate, sodium stearate, magnesium stearate, sodium benzoate, sodium PLKtate, sodium chloride and the like.

Preservatives, stabilizers, dyes and even flavoring agents may be provided in the pharmaceutical composition. Examples of preservatives include sodium benzoate, sorbic acid and esters of p-hydroxybenzoic acid. Antioxidants and suspending agents may be also used.

SALTS/ESTERS

The PLK modulators or candidate compounds of the present invention can be present as salts or esters, in particular pharmaceutically acceptable salts or esters.

Pharmaceutically acceptable salts of the PLK modulators or candidate compounds of the invention include suitable acid addition or base salts thereof. A review of suitable pharmaceutical salts may be found in Berge et al, J Pharm Sci, 66, 1-19 (1977). Salts are formed, for example with strong inorganic acids such as mineral acids, e.g. sulphuric acid, phosphoric acid or hydrohalic acids; with strong organic carboxylic acids, such as alkanecarboxylic acids of 1 to 4 carbon atoms which are unsubstituted or substituted (e.g., by halogen), such as acetic acid; with saturated or unsaturated dicarboxylic acids, for example oxalic, malonic, succinic, maleic, fumaric, phthalic or tetraphthalic; with hydroxycarboxylic acids, for example ascorbic, glycolic, lactic, malic, tartaric or citric acid; with aminoacids, for example aspartic or glutamic acid; with benzoic acid; or with organic sulfonic acids, such as (C_1-C_4)-alkyl- or aryl-sulfonic acids which are unsubstituted or substituted (for example, by a halogen) such as methane- or p-toluene sulfonic acid.

Esters are formed either using organic acids or alcohols/hydroxides, depending on the functional group being esterified. Organic acids include carboxylic acids, such as alkanecarboxylic acids of 1 to 12 carbon atoms which are unsubstituted or substituted (e.g., by halogen), such as acetic acid; with saturated or unsaturated dicarboxylic acid;

sulfonic acid. Suitable hydroxides include inorganic hydroxides, such as sodium hydroxide, potassium hydroxide, calcium hydroxide, aluminium hydroxide. Alcohols include alkanealcohols of 1-12 carbon atoms which may be unsubstituted or substituted, e.g. by a halogen).

ENANTIOMERS/TAUTOMERS

In all aspects of the present invention previously discussed, the invention includes, where appropriate all enantiomers and tautomers of the PLK modulators or candidate compounds of the invention. The man skilled in the art will recognise compounds that possess an optical properties (one or more chiral carbon atoms) or tautomeric characteristics. The corresponding enantiomers and/or tautomers may be isolated/prepared by methods known in the art.

STEREO AND GEOMETRIC ISOMERS

Some of the PLK modulators or candidate compounds of the invention may exist as stereoisomers and/or geometric isomers, e.g. they may possess one or more asymmetric and/or geometric centres and so may exist in two or more stereoisomeric and/or geometric forms. The present invention contemplates the use of all the individual stereoisomers and geometric isomers of those agents, and mixtures thereof. The terms used in the claims encompass these forms, provided said forms retain the appropriate functional activity (though not necessarily to the same degree).

The present invention also includes all suitable isotopic variations of the PLK modulators or candidate compounds, or pharmaceutically acceptable salts thereof. An isotopic variation of a PLK modulator or candidate compound of the present invention or a pharmaceutically acceptable salt thereof is defined as one in which at least one atom is replaced by an atom having the same atomic number but an atomic mass different from the atomic mass usually found in nature. Examples of isotopes that can be incorporated into the agent and pharmaceutically acceptable salts thereof include isotopes of hydrogen, carbon, nitrogen, oxygen, phosphorus, sulphur, fluorine and chlorine such as ^{2}H, ^{3}H, ^{13}C, ^{14}C, ^{15}N, ^{17}O, ^{18}O, ^{31}P, ^{32}P, ^{35}S, ^{18}F and ^{36}Cl, respectively. Certain isotopic variations of the agent and pharmaceutically acceptable salts thereof,

for example, those in which a radioactive isotope such as ^{3}H or ^{14}C is incorporated, are useful in drug and/or substrate tissue distribution studies. Tritiated, i.e., ^{3}H, and carbon-14, i.e., ^{14}C, isotopes are particularly preferred for their ease of preparation and detectability. Further, substitution with isotopes such as deuterium, i.e., ^{2}H, may afford certain therapeutic advantages resulting from greater metabolic stability, for example, increased *in vivo* half-life or reduced dosage requirements and hence may be preferred in some circumstances. Isotopic variations of the PLK modulators or candidate compounds of the present invention can generally be prepared by conventional procedures using appropriate isotopic variations of suitable reagents.

SOLVATES

The present invention also includes solvate forms of the PLK modulators or candidate compounds. The terms used in the claims encompass these forms.

POLYMORPHS

The invention furthermore relates to PLK modulators or candidate compounds of the present invention in their various crystalline forms, polymorphic forms and (an)hydrous forms. It is well established within the pharmaceutical industry that chemical compounds may be isolated in any of such forms by slightly varying the method of purification and or isolation form the solvents used in the synthetic preparation of such compounds.

PRODRUGS

The invention further includes PLK modulators or candidate compounds of the present invention in prodrug form. Such prodrugs are generally compounds of the invention wherein one or more appropriate groups have been modified such that the modification may be reversed upon administration to a human or mammalian subject. Such

THERAPEUTIC USE

The PLK modulators or candidate compounds of the present invention have been found to possess anti-proliferative activity and are therefore believed to be of use in the treatment of proliferative disorders, such as cancers, leukaemias or other disorders associated with uncontrolled cellular proliferation such as psoriasis and restenosis.

A further aspect of the invention therefore relates to a method of treating a proliferative disorder, said method comprising administering to a subject in need thereof a compound selected from the following:

(i) 5'-thioadenosine, or a derivative thereof;

(ii) staurosporine, or a derivative thereof; and

(iii) 4-[4-(4-methyl-2-methylaminothiazol-5-yl)-pyrimidin-2-ylamino]-phenol, 4-[4-(2,4-dimethylthiazol-5-yl)-pyrimidin-2-ylamino]-phenol or 4-[4-(2-amino-4-methyl thiazol-5-yl)-pyrimidin-2-ylamino]-phenol;

or a pharmaceutically acceptable salt thereof, in an amount sufficient to inhibit PLK such that said proliferative disorder is treated.

Another aspect relates to a method of treating a proliferative disorder comprising inhibiting PLK by administering to a subject in need thereof, a therapeutically effective amount of a compound selected from the following:

(i) 5'-thioadenosine, or a derivative thereof;

(ii) staurosporine, or a derivative thereof; and

(iii) 4-[4-(4-methyl-2-methylaminothiazol-5-yl)-pyrimidin-2-ylamino]-phenol, 4-[4-(2,4-dimethyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol or 4-[4-(2-amino-4-methyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol;

or a pharmaceutically acceptable salt thereof, such that treatment of the proliferative disorder occurs.

Another aspect of the invention relates to a method of preventing and/or treating a PLK related disorder comprising administering a PLK modulator or candidate compound of the invention and/or a pharmaceutical composition according to the invention, wherein said

PLK modulator, said candidate compound or said pharmaceutical, is capable of causing a beneficial preventative and/or therapeutic effect.

Preferably, for this aspect, the PLK modulator or candidate compound is selected from the following:

(i) 5'-thioadenosine, or a derivative thereof:

(ii) staurosporine, or a derivative thereof; and

(iii) 4-[4-(4-methyl-2-methylaminothiazol-5-yl)-pyrimidin-2-ylamino]-phenol, 4-[4-(2,4-dimethyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol or 4-[4-(2-amino-4-methyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol;

or a pharmaceutically acceptable salt thereof.

A further aspect of the invention relates to the use of a PLK modulator or candidate compound according to the invention in the preparation of a medicament for treating a PLK related disorder. Preferably, the PLK related disorder is a proliferative disorder, more preferably cancer.

As used herein the phrase "preparation of a medicament" includes the use of the compound directly as the medicament in addition to its use in a screening programme for further therapeutic agents or in any stage of the manufacture of such a medicament.

Another aspect relates to a method of treating a PLK dependent disorder in a subject in need thereof, said method comprising administering to said subject a compound selected from the following:

(i) 5'-thioadenosine, or a derivative thereof;

(ii) staurosporine, or a derivative thereof; and

(iii) 4-[4-(4-methyl-2-methylaminothiazol-5-yl)-pyrimidin-2-ylamino]-phenol, 4-[4-

Preferably, the PLK dependent disorder is a disorder associated with increased PLK activity. Even more preferably, the disorder is cancer.

The term "proliferative disorder" is used herein in a broad sense to include any disorder that requires control of the cell cycle, for example cardiovascular disorders such as restenosis and cardiomyopathy, auto-immune disorders such as glomerulonephritis and rheumatoid arthritis, dermatological disorders such as psoriasis, anti-inflammatory, anti-fungal, antiparasitic disorders such as malaria, emphysema and alopecia. In these disorders, the compounds of the present invention may induce apoptosis or maintain stasis within the desired cells as required.

Preferably, the proliferative disorder is a cancer or leukaemia.

In another preferred embodiment, the proliferative disorder is psoriasis.

The compounds of the invention may inhibit any of the steps or stages in the cell cycle, for example, formation of the nuclear envelope, exit from the quiescent phase of the cell cycle (G0), G1 progression, chromosome decondensation, nuclear envelope breakdown, START, initiation of DNA replication, progression of DNA replication, termination of DNA replication, centrosome duplication, G2 progression, activation of mitotic or meiotic functions, chromosome condensation, centrosome separation, microtubule nucleation, spindle formation and function, interactions with microtubule motor proteins, chromatid separation and segregation, inactivation of mitotic functions, formation of contractile ring, and cytokinesis functions. In particular, the compounds of the invention may influence certain gene functions such as chromatin binding, formation of replication complexes, replication licensing, phosphorylation or other secondary modification activity, proteolytic degradation, microtubule binding, actin binding, septin binding, microtubule organising centre nucleation activity and binding to components of cell cycle signalling pathways.

As defined herein, an anti-proliferative effect within the scope of the present invention may be demonstrated by the ability to inhibit cell proliferation in an *in vitro* whole cell

assay, for example using any of the cell lines A549, HeLa, HT-29, MCF7, Saos-2, CCRF-CEM, HL-60 and K-562, or by showing kinase inhibition in an appropriate assay. These assays, including methods for their performance, are described in more detail in the accompanying Examples. Using such assays it may be determined whether a compound is anti-proliferative in the context of the present invention.

In one preferred embodiment, the compound of the invention is administered orally.

In one embodiment of the invention, the compound of the invention is administered in an amount sufficient to inhibit at least one PLK enzyme.

In a more preferred embodiment of the invention, the compound of the invention is administered in an amount sufficient to inhibit PLK1.

In one particularly preferred embodiment, the compounds of the invention are ATP-antagonistic inhibitors of PLK1.

In the present context ATP antagonism refers to the ability of an inhibitor compound to diminish or prevent PLK catalytic activity, i.e. phosphotransfer from ATP to a macromolecular PLK substrate, by virtue of reversibly or irreversibly binding at the enzyme's active site in such a manner as to impair or abolish ATP binding.

In another preferred embodiment, the compound of the invention is administered in an amount sufficient to inhibit PLK2 and/or PLK3.

Yet another aspect relates to a method of inhibiting PLK in a cell comprising contacting said cell with an amount of a compound selected from the following:

or a pharmaceutically acceptable salt thereof, such that PLK is inhibited in said cell.

Preferably, the cell is a cancer cell.

ADMINISTRATION

The pharmaceutical compositions of the present invention may be adapted for oral, rectal, vaginal, parenteral, intramuscular, intraperitoneal, intraarterial, intrathecal, intrabronchial, subcutaneous, intradermal, intravenous, nasal, buccal or sublingual routes of administration.

For oral administration, particular use is made of compressed tablets, pills, tablets, gellules, drops, and capsules. Preferably, these compositions contain from 1 to 250 mg and more preferably from 10-100 mg, of active ingredient per dose.

Other forms of administration comprise solutions or emulsions which may be injected intravenously, intraarterially, intrathecally, subcutaneously, intradermally, intraperitoneally or intramuscularly, and which are prepared from sterile or sterilisable solutions. The pharmaceutical compositions of the present invention may also be in form of suppositories, pessaries, suspensions, emulsions, lotions, ointments, creams, gels, sprays, solutions or dusting powders.

An alternative means of transdermal administration is by use of a skin patch. For example, the active ingredient can be incorporated into a cream consisting of an aqueous emulsion of polyethylene glycols or liquid paraffin. The active ingredient can also be incorporated, at a concentration of between 1 and 10% by weight, into an ointment consisting of a white wax or white soft paraffin base together with such stabilisers and preservatives as may be required.

Injectable forms may contain between 10 - 1000 mg, preferably between 10 - 250 mg, of active ingredient per dose.

Compositions may be formulated in unit dosage form, i.e., in the form of discrete portions containing a unit dose, or a multiple or sub-unit of a unit dose.

DOSAGE

A person of ordinary skill in the art can easily determine an appropriate dose of one of the instant compositions to administer to a subject without undue experimentation. Typically, a physician will determine the actual dosage which will be most suitable for an individual patient and it will depend on a variety of factors including the activity of the specific compound employed, the metabolic stability and length of action of that compound, the age, body weight, general health, sex, diet, mode and time of administration, rate of excretion, drug combination, the severity of the particular condition, and the individual undergoing therapy. The dosages disclosed herein are exemplary of the average case. There can of course be individual instances where higher or lower dosage ranges are merited, and such are within the scope of this invention.

Depending upon the need, the agent may be administered at a dose of from 0.01 to 30 mg/kg body weight, such as from 0.1 to 10 mg/kg, more preferably from 0.1 to 1 mg/kg body weight.

In an exemplary embodiment, one or more doses of 10 to 150 mg/day will be administered to the patient for the treatment of malignancy.

PLK FRAGMENT

Another aspect of the invention relates to a fragment of PLK, or a homologue, mutant, or derivative thereof, comprising a ligand binding domain, said ligand binding domain being defined by the amino acid residue structural coordinates selected from one or

As used herein, the term "portion thereof" means the structural co-ordinates corresponding to a sufficient number of amino acid residues of the PLK sequence (or homologue thereof) that are capable of interacting with a candidate compound capable of binding to the LBD. This term includes ligand binding domain amino acid residues having amino acid residues from about 4Å to about 5Å of a bound compound or fragment thereof. Thus, for example, the structural co-ordinates provided in the homology model may contain a subset of the amino acid residues in the LBD which may be useful in the modelling and design of compounds that bind to the LBD.

In one preferred embodiment, the fragment of PLK, or a homologue, mutant or derivative thereof, corresponds to a portion of the structure co-ordinates of Table 2.

Another aspect of the invention relates to the use of the above-described fragment of PLK, or a homologue, mutant, or derivative thereof, in an assay for identifying candidate compounds capable of modulating PLK.

The PLK proteins produced by a host recombinant cell may be secreted or may be contained intracellularly depending on the nucleotide sequence and/or the vector used.

As will be understood by those skilled in the art, expression vectors containing a PLK encoding nucleotide sequence or a mutant, variant, homologue, derivative or fragment thereof, may be designed with signal sequences which direct secretion of the PLK coding sequences through a particular prokaryotic or eukaryotic cell membrane.

The PLK encoding sequence may be fused (eg. ligated) to nucleotide sequences encoding a polypeptide domain which will facilitate purification of soluble proteins (Kroll *DJ et al* (1993) DNA Cell Biol 12:441-53). Preferably, the polypeptide domain which facilitates purification of soluble proteins is fused in frame with the PLK encoding sequence. Such purification facilitating domains include, but are not limited to, metal chelating peptides – such as histidine-tryptophan modules that allow purification on immobilised metals (Porath J (1992) Protein Expr Purif 3, 263-281), protein A domains that allow purification on immobilised immunoglobulin, and the domain utilised in the FLAGS extension/affinity

purification system (Immunex Corp, Seattle, WA). The inclusion of a cleavable linker sequence such as Factor XA or enterokinase (Invitrogen, San Diego, CA) between the purification domain and PLK is useful to facilitate purification.

NUCLEOTIDE SEQUENCES

As used herein, the term "nucleotide sequence" refers to nucleotide sequences, oligonucleotide sequences, polynucleotide sequences and variants, homologues, fragments and derivatives thereof (such as portions thereof) which comprise the nucleotide sequences encoding PLK.

The nucleotide sequence may be DNA or RNA of genomic or synthetic or recombinant origin, which may be double-stranded or single-stranded whether representing the sense or antisense strand or combinations thereof.

Preferably, the term nucleotide sequence is prepared by use of recombinant DNA techniques (e.g. recombinant DNA). The nucleotide sequences may include within them synthetic or modified nucleotides. A number of different types of modification to oligonucleotides are known in the art. These include methylphosphonate and phosphorothioate backbones, addition of acridine or polylysine chains at the 3' and/or 5' ends of the molecule. For the purposes of the present invention, it is to be understood that the nucleotide sequences described herein may be modified by any method available in the art.

It will be understood by a skilled person that numerous different nucleotide sequences can encode the same protein as a result of the degeneracy of the genetic code. In addition, it is to be understood that skilled persons may, using routine techniques, make nucleotide substitutions that do not substantially affect the activity encoded by the

a functional protein according to the present invention (or even a modulator of PLK according to the present invention if said modulator comprises a nucleotide sequence or an amino acid sequence).

AMINO ACID SEQUENCES

As used herein, the term "amino acid sequence" is synonymous with the term "polypeptide" and/or the term "protein". In some instances, the term "amino acid sequence" is synonymous with the term "peptide".

The amino acid sequence may be isolated from a suitable source, or it may be made synthetically or it may be prepared by use of recombinant DNA techniques.

VARIANTS/HOMOLOGUES/DERIVATIVES/FRAGMENTS

The PLK described herein is intended to include any polypeptide, which has the activity of the naturally occurring PLK and includes all vertebrate and mammalian forms. Such terms also include polypeptides that differ from naturally occurring forms of PLK by having amino acid deletions, substitutions, and additions, but which retain the activity of PLK.

The term "variant" is used to mean a naturally occurring polypeptide or nucleotide sequences which differs from a wild-type or a native sequence.

The term "fragment" indicates that a polypeptide or nucleotide sequence comprises a fraction of a wild-type or a native sequence. It may comprise one or more large contiguous sections of sequence or a plurality of small sections. The sequence may also comprise other elements of sequence, for example, it may be a fusion protein with another protein. Preferably the sequence comprises at least 50%, more preferably at least 65%, more preferably at least 80%, most preferably at least 90% of the wild-type sequence.

The present invention also encompasses the use of variants, homologues and derivatives of nucleotide and amino acid sequences. Here, the term "homologue" means an entity

having a certain homology with amino acid sequences or nucleotide sequences. Here, the term "homology" can be equated with "identity".

In the present context, an homologous sequence is taken to include an amino acid sequence which may be at least 75, 85 or 90% identical, preferably at least 95 or 98% identical to the subject sequence. Although homology can also be considered in terms of similarity (i.e. amino acid residues having similar chemical properties/functions), it is preferred to express homology in terms of sequence identity.

An homologous sequence is taken to include a nucleotide sequence which may be at least 75, 85 or 90% identical, preferably at least 95 or 98% identical to the subject sequence.

Homology comparisons can be conducted by eye, or more usually, with the aid of readily available sequence comparison programs. These commercially available computer programs can calculate % homology between two or more sequences.

% homology may be calculated over contiguous sequences, i.e. one sequence is aligned with the other sequence and each amino acid in one sequence is directly compared with the corresponding amino acid in the other sequence, one residue at a time. This is called an "ungapped" alignment. Typically, such ungapped alignments are performed only over a relatively short number of residues.

Although this is a very simple and consistent method, it fails to take into consideration that, for example, in an otherwise identical pair of sequences, one insertion or deletion will cause the following amino acid residues to be put out of alignment, thus potentially resulting in a large reduction in % homology when a global alignment is performed.

However, these more complex methods assign "gap penalties" to each gap that occurs in the alignment so that, for the same number of identical amino acids, a sequence alignment with as few gaps as possible - reflecting higher relatedness between the two compared sequences - will achieve a higher score than one with many gaps. "Affine gap costs" are typically used that charge a relatively high cost for the existence of a gap and a smaller penalty for each subsequent residue in the gap. This is the most commonly used gap scoring system. High gap penalties will of course produce optimised alignments with fewer gaps. Most alignment programs allow the gap penalties to be modified. However, it is preferred to use the default values when using such software for sequence comparisons. For example when using the GCG Wisconsin Bestfit package the default gap penalty for amino acid sequences is -12 for a gap and -4 for each extension.

Calculation of maximum % homology therefore firstly requires the production of an optimal alignment, taking into consideration gap penalties. A suitable computer program for carrying out such an alignment is the GCG Wisconsin Bestfit package (University of Wisconsin, U.S.A.; Devereux *et al.*, 1984, Nucleic Acids Research 12:387). Examples of other software than can perform sequence comparisons include, but are not limited to, the BLAST package (see Ausubel *et al.*, 1999 ibid – Chapter 18), FASTA (Atschul *et al.*, 1990, J. Mol. Biol., 403-410) and the GENEWORKS suite of comparison tools. Both BLAST and FASTA are available for offline and online searching (see Ausubel *et al.*, 1999 ibid, pages 7-58 to 7-60). However, for some applications, it is preferred to use the GCG Bestfit program. A new tool, called BLAST 2 Sequences is also available for comparing protein and nucleotide sequence (see *FEMS Microbiol Lett* 1999 174(2): 247-50; *FEMS Microbiol Lett* 1999 177(1): 187-8)

Although the final % homology can be measured in terms of identity, the alignment process itself is typically not based on an all-or-nothing pair comparison. Instead, a scaled similarity score matrix is generally used that assigns scores to each pairwise comparison based on chemical similarity or evolutionary distance. An example of such a matrix commonly used is the BLOSUM62 matrix - the default matrix for the BLAST suite of programs. GCG Wisconsin programs generally use either the public default

values or a custom symbol comparison table if supplied (see user manual for further details). For some applications, it is preferred to use the public default values for the GCG package, or in the case of other software, the default matrix, such as BLOSUM62. Once the software has produced an optimal alignment, it is possible to calculate % homology, preferably % sequence identity. The software typically does this as part of the sequence comparison and generates a numerical result.

The sequences may also have deletions, insertions or substitutions of amino acid residues, which produce a silent change and result in a functionally equivalent substance. Deliberate amino acid substitutions may be made on the basis of similarity in polarity, charge, solubility, hydrophobicity, hydrophilicity, and/or the amphipathic nature of the residues as long as the secondary binding activity of the substance is retained. For example, negatively charged amino acids include aspartic acid and glutamic acid; positively charged amino acids include lysine and arginine; and amino acids with uncharged polar head groups having similar hydrophilicity values include leucine, isoleucine, valine, glycine, alanine, asparagine, glutamine, serine, threonine, phenylalanine, and tyrosine.

Conservative substitutions may be made, for example according to the Table below. Amino acids in the same block in the second column and preferably in the same line in the third column may be substituted for each other:

ALIPHATIC	Non-polar	G A P
		I L V
	Polar - uncharged	C S T M
		N Q
	Polar - charged	D E

occur i.e. like-for-like substitution such as basic for basic, acidic for acidic, polar for polar etc. Non-homologous substitution may also occur i.e. from one class of residue to another or alternatively involving the inclusion of unnatural amino acids such as ornithine (hereinafter referred to as Z), diaminobutyric acid ornithine (hereinafter referred to as B), norleucine ornithine (hereinafter referred to as O), pyriylalanine, thienylalanine, naphthylalanine and phenylglycine.

Replacements may also be made by unnatural amino acids include; alpha* and alpha-disubstituted* amino acids, N-alkyl amino acids*, lactic acid*, halide derivatives of natural amino acids such as trifluorotyrosine*, p-Cl-phenylalanine*, p-Br-phenylalanine*, p-I-phenylalanine*, L-allyl-glycine*, ß-alanine*, L-α-amino butyric acid*, L-γ-amino butyric acid*, L-α-amino isobutyric acid*, L-ε-amino caproic acid#, 7-amino heptanoic acid*, L-methionine sulfone#*, L-norleucine*, L-norvaline*, p-nitro-L-phenylalanine*, L-hydroxyproline#, L-thioproline*, methyl derivatives of phenylalanine (Phe) such as 4-methyl-Phe*, pentamethyl-Phe*, L-Phe (4-amino)#, L-Tyr (methyl)*, L-Phe (4-isopropyl)*, L-Tic (1,2,3,4-tetrahydroisoquinoline-3-carboxyl acid)*, L-diaminopropionic acid # and L-Phe (4-benzyl)*. The notation * has been utilised for the purpose of the discussion above (relating to homologous or non-homologous substitution), to indicate the hydrophobic nature of the derivative whereas # has been utilised to indicate the hydrophilic nature of the derivative, #* indicates amphipathic characteristics.

The term "derivative" or "derivatised" as used herein includes chemical modification of an entity, such as candidate compound or a PLK modulator. Illustrative of such chemical modifications would be replacement of hydrogen by a halo group, an alkyl group, an acyl group or an amino group.

Variant amino acid sequences may include suitable spacer groups that may be inserted between any two amino acid residues of the sequence including alkyl groups such as methyl, ethyl or propyl groups in addition to amino acid spacers such as glycine or β-alanine residues. A further form of variation, involves the presence of one or more amino acid residues in peptoid form, will be well understood by those skilled in the art. For the avoidance of doubt, "the peptoid form" is used to refer to variant amino acid

residues wherein the α-carbon substituent group is on the residue's nitrogen atom rather than the α-carbon. Processes for preparing peptides in the peptoid form are known in the art, for example Simon RJ et al., PNAS (1992) 89(20), 9367-9371 and Horwell DC, Trends Biotechnol. (1995) 13(4), 132-134.

MUTANT

As used herein, the term "mutant" refers to PLK comprising one or more changes in the wild-type PLK sequence.

The term "mutant" is not limited to amino acid substitutions of the amino acid residues in PLK, but also includes deletions or insertions of nucleotides which may result in changes in the amino acid residues in the amino acid sequence of PLK.

The present invention also enables the solving of the crystal structure of PLK mutants. More particularly, by virtue of the present invention, the location of the active site of PLK based on the structural coordinates of Table 2 permits the identification of desirable sites for mutation. For example, one or more mutations may be directed to a particular site - such as the active site - or combination of sites of PLK. Similarly, only a location on, at or near the enzyme surface may be replaced, resulting in an altered surface charge of one or more charge units, as compared to the wild-type enzyme. Alternatively, an amino acid residue in PLK may be chosen for replacement based on its hydrophilic or hydrophobic characteristics.

Such mutants may be characterised by any one of several different properties as compared with wild-type PLK. For example, such mutants may have altered surface charge of one or more charge units, or have an increased stability to subunit dissociation, or an altered substrate specificity in comparison with, or a higher specific

may be generated by site specific replacement of a particular amino acid with an unnaturally occurring amino acid. This may be achieved by growing a host organism capable of expressing either the wild-type or mutant polypeptide on a growth medium depleted of one or more natural amino acids but enriched in one or more corresponding unnaturally occurring amino acids.

HOST CELLS

As used herein, the term "host cell" refers to any cell that comprises nucleotide sequences that are of use in the present invention, for example, nucleotide sequences encoding PLK.

Host cells may be transformed or transfected with a nucleotide sequence contained in a vector e.g. a cloning vector. Preferably, said nucleotide sequence is carried in a vector for the replication and/or expression of the nucleotide sequence. The cells will be chosen to be compatible with the said vector and may for example be prokaryotic (for example bacterial), fungal, yeast or plant cells.

The gram-negative bacterium *E. coli* is widely used as a host for cloning nucleotide sequences. This organism is also widely used for heterologous nucleotide sequence expression. However, large amounts of heterologous protein tend to accumulate inside the cell. Subsequent purification of the desired protein from the bulk of *E. coli* intracellular proteins can sometimes be difficult.

In contrast to *E. coli*, bacteria from the genus Bacillus are very suitable as heterologous hosts because of their capability to secrete proteins into the culture medium. Other bacteria suitable as hosts are those from the genera Streptomyces and Pseudomonas.

Depending on the nature of the polynucleotide and/or the desirability for further processing of the expressed protein, eukaryotic hosts including yeasts or other fungi may be preferred. In general, yeast cells are preferred over fungal cells because yeast cells are easier to manipulate. However, some proteins are either poorly secreted from

the yeast cell, or in some cases are not processed properly (*e.g.* hyperglycosylation in yeast). In these instances, a different fungal host organism should be selected.

Examples of expression hosts are fungi - such as Aspergillus species (such as those described in EP-A-0184438 and EP-A-0284603) and Trichoderma species; bacteria - such as Bacillus species (such as those described in EP-A-0134048 and EP-A-0253455), Streptomyces species and Pseudomonas species; yeasts - such as Kluyveromyces species (such as those described in EP-A-0096430 and EP-A-0301670) and Saccharomyces species; and mammalian cells – such as CHO-K1 cells.

The use of host cells may provide for post-translational modifications as may be needed to confer optimal biological activity on recombinant expression products of the present invention.

Aspects of the present invention also relate to host cells comprising the PLK constructs of the present invention. The PLK constructs may comprise a nucleotide sequence for replication and expression of the sequence. The cells will be chosen to be compatible with the vector and may for example be prokaryotic (for example bacterial), fungal, yeast or plant cells.

In a preferred embodiment, the host cells are mammalian cells, such as CHO-K1 cells.

VECTOR

Aspects of the present invention relate to a vector comprising a nucleotide sequence, such as a nucleotide sequence encoding PLK or a modulator of PLK, administered to a subject.

and by way of example, some vectors used in recombinant DNA techniques allow entities, such as a segment of DNA (such as a heterologous DNA segment, such as a heterologous cDNA segment), to be transferred into a host and/or a target cell for the purpose of replicating the vectors comprising nucleotide sequences and/or expressing the proteins encoded by the nucleotide sequences. Examples of vectors used in recombinant DNA techniques include, but are not limited to, plasmids, chromosomes, artificial chromosomes or viruses.

The term "vector" includes expression vectors and/or transformation vectors.

The term "expression vector" means a construct capable of *in vivo* or *in vitro/ex vivo* expression.

The term "transformation vector" means a construct capable of being transferred from one species to another.

REGULATORY SEQUENCES

In some applications, nucleotide sequences are operably linked to a regulatory sequence which is capable of providing for the expression of the nucleotide sequence, such as by a chosen host cell. By way of example, a vector comprising the PLK nucleotide sequence is operably linked to such a regulatory sequence i.e. the vector is an expression vector.

The term "operably linked" refers to a juxtaposition wherein the components described are in a relationship permitting them to function in their intended manner. A regulatory sequence "operably linked" to a coding sequence is ligated in such a way that expression of the coding sequence is achieved under conditions compatible with the control sequences.

The term "regulatory sequences" includes promoters and enhancers and other expression regulation signals.

The term "promoter" is used in the normal sense of the art, e.g. an RNA polymerase binding site.

Enhanced expression of a nucleotide sequence, for example, a nucleotide sequence encoding PLK, may also be achieved by the selection of heterologous regulatory regions, e.g. promoter, secretion leader and terminator regions, which serve to increase expression and, if desired, secretion levels of the protein of interest from the chosen expression host and/or to provide for the inducible control of the expression of PLK. In eukaryotes, polyadenylation sequences may be operably connected to the PLK nucleotide sequence.

Preferably, the PLK nucleotide sequence is operably linked to at least a promoter.

Aside from the promoter native to the gene encoding the PLK nucleotide sequence, other promoters may be used to direct expression of the PLK polypeptide. The promoter may be selected for its efficiency in directing the expression of the PLK nucleotide sequence in the desired expression host.

In another embodiment, a constitutive promoter may be selected to direct the expression of the PLK nucleotide sequence. Such an expression construct may provide additional advantages since it circumvents the need to culture the expression hosts on a medium containing an inducing substrate.

Hybrid promoters may also be used to improve inducible regulation of the expression construct.

The promoter can additionally include features to ensure or to increase expression in a

light or stress inducible elements. Also, suitable elements to enhance transcription or translation may be present.

EXPRESSION VECTOR

Preferably, nucleotide sequences, such as nucleotide sequences encoding PLK or modulators of PLK, are inserted into a vector that is operably linked to a control sequence that is capable of providing for the expression of the coding sequence by the host cell.

Nucleotide sequences produced by a host recombinant cell may be secreted or may be contained intracellularly depending on the sequence and/or the vector used. As will be understood by those of skill in the art, expression vectors can be designed with signal sequences, which direct secretion of the nucleotide sequence through a particular prokaryotic or eukaryotic cell membrane.

Preferably, the expression vectors are stably expressed in CHO cells as described previously (Ehlers *et al.* (1996) *Biochemistry 35*, 9549-9559). More preferably, the expression vectors are pLEN- tACEΔ36g(1, 2, 3, 4) and pLEN- tACEΔ36g(1,3).

FUSION PROTEINS

PLK or a modulator of PLK may be expressed as a fusion protein to aid extraction and purification and/or delivery of the modulator of PLK or the PLK protein to an individual and/or to facilitate the development of a screen for modulators of PLK.

Examples of fusion protein partners include glutathione-S-transferase (GST), 6xHis, GAL4 (DNA binding and/or transcriptional activation domains) and β-galactosidase.

It may also be convenient to include a proteolytic cleavage site between the fusion protein partner and the protein sequence of interest to allow removal of fusion protein sequences. Preferably, the fusion protein will not hinder the activity of the protein of interest.

The fusion protein may comprise an antigen or an antigenic determinant fused to the substance of the present invention. In this embodiment, the fusion protein may be a non-naturally occurring fusion protein comprising a substance, which may act as an adjuvant in the sense of providing a generalised stimulation of the immune system. The antigen or antigenic determinant may be attached to either the amino or carboxy terminus of the substance.

ORGANISM

The term "organism" in relation to the present invention includes any organism that could comprise PLK and/or modulators of PLK. Examples of organisms may include mammals, fungi, yeast or plants.

Preferably, the organism is a mammal. More preferably, the organism is a human.

TRANSFORMATION

As indicated earlier, the host organism can be a prokaryotic or a eukaryotic organism. Examples of suitable prokaryotic hosts include *E. coli* and *Bacillus subtilis*. Teachings on the transformation of prokaryotic hosts are well documented in the art, for example see Sambrook et al (Molecular Cloning: A Laboratory Manual, 2nd edition, 1989, Cold Spring Harbor Laboratory Press) and Ausubel *et al.*, Current Protocols in Molecular Biology (1995), John Wiley & Sons, Inc. Examples of suitable eukaryotic hosts include mammalian cells.

If a prokaryotic host is used then the nucleotide sequence, such as the PLK nucleotide sequence, may need to be suitably modified before transformation - such as by removal of introns.

The present invention also relates to the transformation of a host cell with a

sequence and/or the vector used. As will be understood by those of skill in the art, expression vectors containing coding sequences can be designed with signal sequences which direct secretion of the coding sequences through a particular prokaryotic or eukaryotic cell membrane. Other recombinant constructions may join the coding sequence to nucleotide sequence encoding a polypeptide domain, which will facilitate purification of soluble proteins (Kroll *DJ et al* (1993) DNA Cell Biol 12:441-53) e.g. 6-His or Glutathione-*S*-transferase.

TRANSFECTION

Vectors comprising for example, the PLK nucleotide sequence, may be introduced into host cells, for example, mammalian cells, using a variety of methods.

Typical transfection methods include electroporation, DNA biolistics, lipid-mediated transfection, compacted DNA-mediated transfection, liposomes, immunoliposomes, lipofectin, cationic agent-mediated, cationic facial amphiphiles (CFAs) (*Nature Biotech.* (1996) 14, 556), multivalent cations such as spermine, cationic lipids or polylysine, 1, 2,-bis (oleoyloxy)-3-(trimethylammonio) propane (DOTAP)-cholesterol complexes (Wolff and Trubetskoy 1998 Nature Biotechnology 16: 421) and combinations thereof.

Uptake of nucleic acid constructs by mammalian cells is enhanced by several known transfection techniques for example those including the use of transfection agents. Example of these agents include cationic agents (for example calcium phosphate and DEAE-dextran) and lipofectants (for example lipofectam™ and transfectam™). Typically, nucleic acid constructs are mixed with the transfection agent to produce a composition.

Such methods are described in many standard laboratory manuals - such as Sambrook *et al.*, Molecular Cloning: A Laboratory Manual, 2d ed. (1989) Cold Spring Harbor Laboratory Press, Cold Spring Harbor, N.Y.

The present invention is further described by way of example, and with reference to the following figures wherein:

Figure 1 shows multiple sequence alignment (Clustal W) of human PLK1 (P53350), PLK2 (Q9NYY3), and PLK3 (Q9H4B4).

Figure 2 shows a schematic view of PLK1 homology model in complex with ATP (stick model, labelled). The protein structure is indicated with a ribbon (loops, thin; helices, thick; sheets, arrows). The Cys residues are shown with space-filled atoms and are labelled.

Figure 3 shows sequence alignment of PLK1 and PKA kinase domains.

Figure 4 shows modelled complex between PLK1 and ATP (a) and 5'-thioadenosine (b). The positions of the thiol groups (SH) of Cys^{67} and 5'thioadenosine are indicated.

Figure 5 shows dose response curves of PLK1 activity inhibition by various adenosine derivatives in the absence or presence of the reducing agent dithiothreitol (+DTT or – DTT).

Figure 6 shows kinetic analysis of PLK1 inhibition by 5'-thioadenosine.

Figure 7 shows modelled PLK1-bound conformations of ATP (a); 5'-thioadenosine (b); staurosporine (c); and 4-[4-(4-methyl-2-methylamino-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol (d). Non-H atoms are labelled.

EXAMPLES

Such techniques are explained in the literature. See, for example, J. Sambrook, E. F. Fritsch, and T. Maniatis, 1989, *Molecular Cloning: A Laboratory Manual*, Second Edition, Books 1-3, Cold Spring Harbor Laboratory Press; Ausubel, F. M. et al. (1995 and periodic supplements; *Current Protocols in Molecular Biology*, ch. 9, 13, and 16, John Wiley & Sons, New York, N.Y.); B. Roe, J. Crabtree, and A. Kahn, 1996, *DNA Isolation and Sequencing: Essential Techniques*, John Wiley & Sons; J. M. Polak and James O'D. McGee, 1990, *In Situ Hybridization: Principles and Practice*; Oxford University Press; M. J. Gait (Editor), 1984, *Oligonucleotide Synthesis: A Practical Approach*, Irl Press; D. M. J. Lilley and J. E. Dahlberg, 1992, *Methods of Enzymology: DNA Structure Part A: Synthesis and Physical Analysis of DNA* Methods in Enzymology, Academic Press; Using Antibodies : A Laboratory Manual : Portable Protocol NO. I by Edward Harlow, David Lane, Ed Harlow (1999, Cold Spring Harbor Laboratory Press, ISBN 0-87969-544-7); Antibodies : A Laboratory Manual by Ed Harlow (Editor), David Lane (Editor) (1988, Cold Spring Harbor Laboratory Press, ISBN 0-87969-314-2), 1855. Handbook of Drug Screening, edited by Ramakrishna Seethala, Prabhavathi B. Fernandes (2001, New York, NY, Marcel Dekker, ISBN 0-8247-0562-9); and Lab Ref: A Handbook of Recipes, Reagents, and Other Reference Tools for Use at the Bench, Edited Jane Roskams and Linda Rodgers, 2002, Cold Spring Harbor Laboratory, ISBN 0-87969-630-3. Each of these general texts is herein incorporated by reference.

Example 1

Construction of PLK1 homology model

The homology model for PLK1 kinase domain was generated using the program module Homology within the molecular modelling package Insight II (Accelrys, San Diego, CA) [38]. The sequence containing the kinase domain of PLK1 (residues 1 – 356) was employed in a FASTA sequence and structural search [39] in order to find the closest sequence-related kinase for which experimental structural information was available. For this search, the BLOSUM 50 scoring matrix [40] and a specific residue string value of 2 was employed. The closest match of known structure proved to be that of cAMP-dependent protein kinase (protein kinase A, PKA) with a sequence identity of

30 % and similarity of close to 50 % (*Figure 3*). Although these values are typically low for homology model building, the structural conservation of protein kinases was thought to allow a valid structure to be generated. Sequence alignment of PLK1 kinase domain with PKA in addition to CDK2 and ERK2 (which also were among the most homologous structures) indicated that the minimal kinase domain included residues 52 – 308. For the sequence alignment, the PAM 120 multiple scoring matrix [41] was used with a dimension block of 0.6, a high significance p value of 0.0001, a not significant p value of 0.1, and a pair-wise threshold of 60. Using a combination of the three structures to generate coordinates for the regions that had the highest identity in each kinase (*Table 1*), a model structure for the kinase domain was constructed. The strategy generally involved using PKA to define the structurally conserved regions (SCRs) from which the coordinates were subsequently transferred. This was then followed by loop construction where the non-SCRs were generated by *de-novo* building and subsequent evaluation of the most realistic coordinates (in terms of energetics of the loop itself and the exclusion of loops leading to overlapping atoms). After loop building was completed for missing coordinates, the raw coordinates were then refined using successive rounds of end repair splice repairing using an omega force constant of 50, energy minimization (100 steps of steepest descent to a derivative of 5). The model was then completed through using a further minimisation and 1 ps of molecular dynamics to more fully explore the conformational space of the loop regions. The final model structure was then checked against databases of protein structures for bond length and dihedral angle violations. The results indicated that these as a whole were within acceptable limits with > 80 % of residues having phi-psi plots with the allowed region in Ramachandran space [42]. The coordinate file for the final PLK1 homology model – ATP complex in Brookhaven Protein Databank (PDB) format [43] is shown in *Table 2*.

Example 2

downstream of the ORF, by inclusion in the antisense PCR primer. The PCR product generated was cloned into pCR4-Topo (Invitrogen), and sequenced. The ORF was then sub-cloned as an Nhe I / Eco RI fragment into pSSP1, a derivative of bacmid transfer vector pFastBac HTa (Invitrogen). The PLK1 ORF was cloned into pSSP1 such that the resulting PLK1 translation product would have a 19 amino acid N-terminal tag (MSYYHHHHHHGMASDDDDK) containing a hexahistidine tag and an enterokinase cleavage site. The pSSP1-Plk1 expression cassette was transferred into bacmid DNA by transposition in E. coli DH10Bac (Invitrogen). Purified recombinant bacmid DNA was transfected into Sf9 cells, to produce an infective stock of recombinant baculovirus. Following subsequent amplification and titering of the baculoviral stock, this was used to infect Sf9 cells at a multiplicity of infection of approximately 3. His-tagged PLK1 was expressed by incubating the infected cells at 27 °C, with shaking. Two days after infection, the cells were collected by centrifugation. Prior to purification, PLK1 expression was confirmed by Western blotting. To the cell pellet from 150 mL Sf9 insect cell culture 10 mL lysis buffer [10 mM Tris-HCl pH 8.0, 150 ml NaCl, 20 mM β-mercaptoethanol, 1 mM PMSF, 1 mM benzamidine, protease inhibitor cocktail (Sigma; 1 : 1,000 diluted), 20 mM imidazole], supplemented with 2 mM NaF and 1 mM Na_3VO_4, was added; the mixture was sonicated (6 × 20 s) on ice and centrifuged for 15 min at 15,000 r.p.m. The supernatant was filtered (0.45 μm filter) and the filtrate was applied to a pre-equilibrated (with 20 mL lysis buffer) 1.2-mL Ni-NTA agarose column (Qiagen). After incubation for 2 h at 4 °C, the non-bound fraction was eluted with was buffer (as lysis buffer but 300 mM NaCl and without imidazole). Protein was eluted with elution buffer (as lysis buffer but 100 mM NaCl, 250 mM imidazole, 0.02 % Nonidet P-40). Pooled fractions containing target protein were applied to an equilibrated (with dialysis buffer) 5-mL HiTrap™ desalting column (Amersham Biosciences) and eluted with dialysis buffer (25 mM Tris/MES pH 7.6, 1 mM β-mercaptoethanol, 0.01 % Tween-20, 10 mM $MgCl_2$, 50 μM ATP, 100 mM NaCl, 1 mM PMSF, 1 mM benzamidine, 10 % glycerol). Pooled fractions containing pure target protein were centrifuged 15,000 r.p.m. for 15 min. The supernatant PLK1 stock solution was stored at –70 °C.

Example 3

PLK1 assay

PLK1 kinase activity was assayed using human CDC25C phosphatase as a substrate [4]. The assays were carried out using 96-well microtitre plates by incubating CDC25C (2 μg/well) with 1 μg/well of purified human recombinant PLK1 and varying concentrations of the candidate compound in a total volume of 25 μL of 20 mM Tris/HCl buffer pH 7.5, supplemented with 25 mM β-glycerophosphate, 5 mM EGTA, 1 mM DTT, and 1 mM $NaVO_3$. Reaction was initiated by the addition of 100 μM ATP and 0.5 μCi of [γ-^{32}P]-ATP. The reaction mixture was incubated at 30 °C for 1 h, then stopped with 75 mM aq orthophosphoric acid, transferred onto a 96-well P81 filter plate (Whatman), dried, and the extent of CDC25C phosphorylation was assessed by scintillation counting using a Packard TopCount plate reader.

Example 4

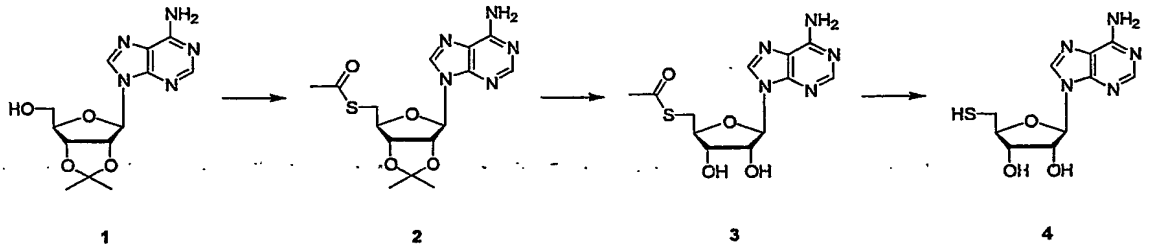
Casein kinase II (CKII) assay

Human recombinant CKII activity was assayed using the peptide H-Arg-Arg-Arg-Glu-Glu-Glu-Thr-Glu-Glu-Glu-OH as a substrate. The assays were carried out using 96-well microtitre plates by incubating the peptide substrate (10 μM) with 20 Units/well of CKII (New England Biolabs) and varying concentrations of the candidate compound in a total volume of 25 μL of 25 mM MOPS buffer pH 7.0, supplemented with 25 mM β-glycerophosphate, 5 mM EGTA, 1 mM DTT, and 1 mM $NaVO_3$. Reaction was initiated by the addition of 100 μM ATP and 0.25 μCi of [γ-^{32}P]-ATP. The reaction mixture was incubated at 30 °C for 15 minutes, then stopped with 75 mM aq orthophosphoric acid, transferred onto a 96-well P81 filter plate (Whatman), dried, and the extent of peptide phosphorylation was assessed by scintillation counting using a Packard TopCount plate reader.

thiazol-5-yl)-pyrimidin-2-ylamino]-phenol were synthesised in accordance with the methodology described in WO 01/72745. Staurosporine and derivatives thereof (such as CGP 41251 and UCN-01) are described in the literature [see for example, Gescher A., Gen Pharmacol. 1998, 31, p721-8].

Synthesis of 5'-deoxy-5-thio-adenosine (4)

5'-Deoxy-5-thio-adenosine (4) is a known compound [45] and it can be prepared readily from commercially available 2',3'-isopropylideneadenosine 1 as shown in *Scheme 1* [46].



Scheme 1

5'-Deoxy-5'-acetylthio-2',3'-O-isopropylideneadenosine (2)

Diethyl azodicarboxyl-ate (3.4 mL, 21.73 mmol) was added drop-wise over 5 min to an ice-cold solution of triphenylphosphine (5.7 g, 21.73 mmol). The solution was stirred for 30 min at 0 °C prior to the addition of 2',3'-*O*-isopropylideneadenosine (1; 3.0 g, 9.76 mmol) and stirring was then continued for a further 10 min to produce a yellow suspension. To the suspension a solution of thioacetic acid (1.6 mL, 21.73 mmol) in absol tetrahydrofuran (5 mL) was added drop-wise and stirring was then continued for a further 1 h at 0 °C. During this time the yellow suspension became a darker yellow solution. After stirring for 1 h the solvent was removed under reduced pressure and the resulting yellowish residue was purified by flash chromatography on silica gel [350 g, $CHCl_3$/THF (4:1 v/v) and then $CHCl_3/CH_3OH$ (9:1 v/v)]. The fractions containing the product were combined and the solvent removed under reduced pressure. The residue was dried *in vacuo* (0.5 mbar) to furnish pure protected thionucleoside 2 (3.2 g, 90 %) as a white foam; TLC R_f (CH_2Cl_2/CH_3OH, 9:1 v/v) = 0.6, mp = 56-57 °C; ^{1}H-NMR ($CDCl_3$): δ 1.39 (s, 6H, CH_3), 2.34 (s, 3H, $COCH_3$), 3.18 and 3.29 (AB part of ABX

spectrum, $J_{5'a\text{-}H,4'\text{-}H} = J_{5'b\text{-}H,4'\text{-}H} = 6.5$ Hz, $J_{gem} = 13.5$ Hz, 2H, 5'a-H, 5'b-H), 4.34 (dt, $J_{4'\text{-}H,3'\text{-}H} = 3$ Hz, $J_{4'a\text{-}H,5a'\text{-}H} = J_{4'\text{-}H,5'b\text{-}H} = 7$ Hz, 1H, 4'-H), 4.97 (dd, $J_{3'\text{-}H,4'\text{-}H} = 3$ Hz, $J_{3'\text{-}H,2'\text{-}H} = 6.5$ Hz, 1H, 3'-H), 5.51 (dd, $J_{2'\text{-}H,1'\text{-}H} = 2$ Hz, $J_{2'\text{-}H,3'\text{-}H} = 6.5$ Hz, 1H, 2'-H), 6.07 (d, $J_{1'\text{-}H,2'\text{-}H} =$ Hz, 1H, 1'-H), 5.9 (s, br., 2H, NH_2), 7.90 (s, 1H, 8-H) and 8.36 (s, 1H, 2-H); ^{13}C-NMR ($CDCl_3$): δ25.56 (q, CH_3), 27.33 (q, CH_3), 30.79 (q, $COCH_3$), 31.60 (t, C-5'), 84.24 (d, C-3'), 84.43 (d, C-2'), 86.47 (d, C-4'), 91.07 (d, C-1'), 114.75 (s, $C(CH_3)_2$), 120.53 (s, C-5), 140.09 (d, C-8), 149.42 (s, C-4), 153.45 (d, C-2), 155.92 (s, C-6) and 194.79 (s, CO); ESMS; *m/z*: 366.0 [M + H$^+$]; $[\alpha]_D$ ($CDCl_3$) = -13.2.

5'-Deoxy-5'acetyl-thioadenosine (3)

A solution of compound **2** (200 mg, 0.54 mmol) was stirred in a mixture of formic acid and water (10 ml, 1:1) at room temperature. The progress of the reaction was monitored by reversed-phase HPLC. After 50 h reaction time the solvent was evaporated under reduced pressure. Traces of formic acid were removed by co-evaporating 5 times with absolute ethanol to produce an off-white powder, which was purified by silica gel flash chromatography [30 g, CH_2Cl_2/CH_3OH (4:1 v/v)]. The fractions containing the product were combined, the solvent removed under reduced pressure and the product further dried *in vacuo* (0.5 mbar) to title compound **3** (150 mg, 86 %); TLC R_f (CH_2Cl_2:CH_3OH, 9:1 v/v) = 0.24; ^{1}H-NMR ($CDCl_3$): δ2.32 (s, 3H, $COCH_3$), 3.15 and 3.34 (AB part of ABX spectrum, $J_{5'\text{-}H,4'\text{-}H} = 5.5$ Hz, $J_{5'b\text{-}H,}$ 4'-H = 7 Hz, $J_{gem} = 14$ Hz, 2H, 5'a-H, 5'b-H), 3.9 (ddd, $J_{4'\text{-}H,3'\text{-}H} = 3.5$ Hz, $J_{5'a\text{-}H,4'\text{-}H} = 6$ Hz, $J_{5'b\text{-}H,4'\text{-}H} = 7.5$ Hz, 1H, 4'-H), 4.08 (m, 1H, 3'-H), 4.76 (t, $J_{2'\text{-}H,1'\text{-}H} = J_{2'\text{-}H,3'\text{-}H} = J_{2'\text{-}H,2'\text{-}OH} = 6$ Hz, 1H, 2'-H), 5.37 (s, 1H, D_20 exchangeable, 3'-OH), 5.51 (s, 1H, D_20 exchangeable, 2'-OH), 5.85 (d, $J_{1'\text{-}H,2'\text{-}H} =$ 6 Hz, 1H, 1'-H), 7.28 (s, br., 2H, D_20 exchangeable, 6-NH_2), 8.14 (s, 1H, 2-H) and 8.53 (s, 1H, 8-H); ESMS; *m/z*: 326.5 [M + H$^+$].

5'-Deoxy-5'-thioadenosine (4)

vacuo to afford title compound 4 (25 mg, 55 %); TLC R_f (CH_2Cl_2/CH_3OH, 7:1 v/v) = 0.85; mp = 109-110 °C, ^{1}H-NMR [(D_6 DMSO)]: δ 2.57 (s, br., 1H, 5'-SH), 2.75-2.80 (m, 2H, 5'a-H, 5'b-H), 3.98 (dt, $J_{4'\text{-H, }3'\text{-H}} = 3$ Hz, $J_{4'\text{-H, }5'a\text{-H}} = J_{4'\text{-H, }5'b\text{-H}} = 6$ Hz, 1H, 4'-H), 4.18 (q, $J_{3'\text{-H, }2'\text{-H}} = J_{3'\text{-H, }4'\text{-H}} = J_{3'\text{-H, }3'\text{-OH}} = 4$ Hz, 1H, 3'-H), 4.78 (q, $J_{2'\text{-H, }1'\text{-H}} = J_{2'\text{-H, }3'\text{-H}} = J_{2'\text{-H, }2'\text{-OH}} = 5$ Hz, 1H, 2'-H), 5.28 (d, $J_{3'\text{-OH, }3'\text{-OH}} = 5$ Hz, 1H, 3'-OH), 5.48 (d, $J_{2'\text{-OH, }2'\text{-H}} = 6$ Hz, 1H, 2'-OH), 5.88 (d, $J_{1'\text{-H, }2'\text{-H}} = 6$ Hz, 1H, 1'-H), 7.28 (s, br., 2H, 6-NH_2), 8.14 (s, 1H, 2-H) and 8.35 (s, 1H, 8-H); ESMS; *m/z*: 283.92 [M + H^+]; $[\alpha]_D$ (DMSO) = -29.3.

Example 6

Inhibition of PLK1 enzymatic activity by adenosine, thioadenosines, and thiol-reactive compounds

Adenosine, N-ethylmaleimide, iodoacetamide, and thimerosal were obtained from Sigma Chemical Co. 2'-Thioadenosine was obtained from Calbiochem. 5'-Thioadenosine was prepared as described in *Example 5*. All compounds were made up as 10 mM stocks in neat dimethylsulfoxide and fresh dilutions to the desired concentrations were made in assay buffer prior to the assay. The candidate compounds were incubated with the enzyme in the kinase assay buffer for the duration of the assay, usually 1 hour at 30 °C (refer *Example 3)*. For each compound duplicate samples, one of which contained dithiothreitol (DTT) at 1 mM final concentration, were assayed. The results are summarized in *Table 3* and *Figure 5*.

Example 7

ATP-dependence of PLK1 inhibition by 5'-thioadenosine

The kinase assay described in *Example 3* was used. ATP dependence of the effects of adenosine, 2'-thioadenosine, 5-'thioadenosine, and thimerosal was investigated at 12.5, 25, 50, and 100 μM ATP. The results showed that none of these compounds were classical competitive inhibitors with respect to ATP, as would be expected from a covalent inhibitor. Results of the kinetic analysis with 5'-thioadenosine are shown in *Figure 6*.

Example 8

Contact models of PLK1 kinase domain with bound ligands

The homology model described in *Example 1* was used as the basis for the docking of ATP, 5'-thioadenosine, and two additional ATP-competitive kinase inhibitors we have found to inhibit PLK1. The conformations of these ligands in the PLK1 ATP-binding pocket are depicted in *Figure 7*. Descriptions of the PLK1-ligand complex structures in the form of interatomic distances between the residues lining the ATP-binding pocket of PLK1 and the ligands were obtained using the molecular modelling programs Quanta2000 (Accelrys, CA, USA) and Maestro (Schrodinger Inc., Oregon, USA). The output from the former lists all contacts between PLK1 and ligands that are less than 3.5 Å. In the latter case a listing of all PLK1-ligand contacts not involving H atoms is given, together with the interatomic distances. Also given is a measure of the quality of the contacts. Only favourable contacts are listed and the closer the value of the contact cut-off ratio to 1.3, the better the contact. Results are summarized in *Table 4* (Maestro) & *Table 5* (Quanta) for ATP, in *Table 6* (Maestro) & *Table 7* (Quanta) for 5'-thioadenosine, in *Table 8* (Maestro) & *Table 9* (Quanta) for staurosporine, and in *Table 10* (Maestro) & *Table 11* (Quanta) for 4-[4-(4-methyl-2-methylamino-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol. The ligand atom numbering is shown in *Figure 7*.

Various modifications and variations of the invention will be apparent to those skilled in the art without departing from the scope and spirit of the invention. Although the invention has been described in connection with specific preferred embodiments, it should be understood that the invention as claimed should not be unduly limited to such specific embodiments. Indeed, various modifications of the described modes for carrying out the invention which are obvious to those skilled in the relevant fields are intended to be covered by the present invention.

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Table 1. Sequence comparison between PLK1 and CDK2, ERK-2, or PKA kinase domains, respectively.

PLK1 sequence segment	Sequence identity (%)		
	CDK2	*ERK-2*	*PKA*
1–50	0	8	12
51–100	14	20	28
101–150	18	8	20
151–200	44	48	44
201–250	30	30	42
251–306	18	20	22

Table 2. PDB coordinate file of PLK1-ATP homology model

```
ATOM      1  N   ARG    52     108.414 117.322  91.897  1.00  0.00           N
ATOM      2  CA  ARG    52     109.182 116.827  90.698  1.00  0.00           C
ATOM      3  C   ARG    52     108.390 116.045  89.578  1.00  0.00           C
ATOM      4  O   ARG    52     108.985 115.798  88.530  1.00  0.00           O
ATOM      5  CB  ARG    52     110.589 116.233  91.053  1.00  0.00           C
ATOM      6  CG  ARG    52     110.801 114.702  91.020  1.00  0.00           C
ATOM      7  CD  ARG    52     112.287 114.328  91.157  1.00  0.00           C
ATOM      8  NE  ARG    52     112.450 112.916  90.739  1.00  0.00           N
ATOM      9  CZ  ARG    52     113.551 112.190  90.870  1.00  0.00           C
ATOM     10  NH1 ARG    52     114.666 112.630  91.370  1.00  0.00           N
ATOM     11  NH2 ARG    52     113.501 110.971  90.474  1.00  0.00           N
ATOM     12 1H   ARG    52     107.626 116.687  92.087  1.00  0.00           H
ATOM     13 2H   ARG    52     109.037 117.350  92.717  1.00  0.00           H
ATOM     14  HE  ARG    52     111.635 112.458  90.308  1.00  0.00           H
ATOM     15  HA  ARG    52     109.432 117.749  90.134  1.00  0.00           H
ATOM     16 1HB  ARG    52     111.303 116.678  90.331  1.00  0.00           H
ATOM     17 2HB  ARG    52     110.945 116.616  92.029  1.00  0.00           H
ATOM     18 1HG  ARG    52     110.209 114.203  91.813  1.00  0.00           H
ATOM     19 2HG  ARG    52     110.408 114.292  90.070  1.00  0.00           H
ATOM     20 1HD  ARG    52     112.925 114.977  90.524  1.00  0.00           H
ATOM     21 2HD  ARG    52     112.620 114.481  92.204  1.00  0.00           H
ATOM     22 2HH1 ARG    52     114.619 113.601  91.675  1.00  0.00           H
ATOM     23 1HH1 ARG    52     115.438 111.966  91.428  1.00  0.00           H
ATOM     24 1HH2 ARG    52     112.572 110.717  90.120  1.00  0.00           H
ATOM     25 2HH2 ARG    52     114.330 110.391  90.596  1.00  0.00           H
ATOM     26  N   TYR    53     107.105 115.659  89.725  1.00  0.00           N
ATOM     27  CA  TYR    53     106.360 114.857  88.698  1.00  0.00           C
ATOM     28  C   TYR    53     104.944 115.448  88.356  1.00  0.00           C
ATOM     29  O   TYR    53     104.213 115.917  89.234  1.00  0.00           O
ATOM     30  CB  TYR    53     106.221 113.387  89.193  1.00  0.00           C
ATOM     31  CG  TYR    53     107.481 112.506  89.105  1.00  0.00           C
ATOM     32  CD1 TYR    53     108.238 112.270  90.254  1.00  0.00           C
ATOM     33  CD2 TYR    53     107.859 111.902  87.899  1.00  0.00           C
ATOM     34  CE1 TYR    53     109.362 111.450  90.197  1.00  0.00           C
ATOM     35  CE2 TYR    53     108.977 111.069  87.849  1.00  0.00           C
ATOM     36  CZ  TYR    53     109.729 110.848  89.000  1.00  0.00           C
ATOM     37  OH  TYR    53     110.838 110.047  88.972  1.00  0.00           O
ATOM     38  H   TYR    53     106.610 115.929  90.587  1.00  0.00           H
ATOM     39  HA  TYR    53     106.932 114.835  87.749  1.00  0.00           H
ATOM     40 1HB  TYR    53     105.807 113.374  90.220  1.00  0.00           H
ATOM     41 2HB  TYR    53     105.431 112.881  88.609  1.00  0.00           H
ATOM     42  HD1 TYR    53     107.971 112.729  91.194  1.00  0.00           H
ATOM     43  HD2 TYR    53     107.294 112.078  86.995  1.00  0.00           H
ATOM     44  HE1 TYR    53     109.966 111.296  91.080  1.00  0.00           H
ATOM     45  HE2 TYR    53     109.268 110.610  86.916  1.00  0.00           H
ATOM     46  HH  TYR    53     111.034 109.782  88.067  1.00  0.00           H
ATOM     47  N   VAL    54     104.539 115.358  87.076  1.00  0.00           N
ATOM     48  CA  VAL    54     103.182 115.765  86.588  1.00  0.00           C
ATOM     49  C   VAL    54     102.488 114.515  85.933  1.00  0.00           C
ATOM     50  O   VAL    54     102.989 113.950  84.954  1.00  0.00           O
```

ATOM	51	CB	VAL	54	103.294	116.991	85.608	1.00	0.00	C
ATOM	52	CG1	VAL	54	101.959	117.391	84.930	1.00	0.00	C
ATOM	53	CG2	VAL	54	103.822	118.277	86.288	1.00	0.00	C
ATOM	54	H	VAL	54	105.247	114.977	86.430	1.00	0.00	H
ATOM	55	HA	VAL	54	102.552	116.097	87.438	1.00	0.00	H
ATOM	56	HB	VAL	54	104.004	116.714	84.802	1.00	0.00	H
ATOM	57	1HG1	VAL	54	101.183	117.679	85.665	1.00	0.00	H
ATOM	58	2HG1	VAL	54	102.083	118.243	84.234	1.00	0.00	H
ATOM	59	3HG1	VAL	54	101.536	116.567	84.325	1.00	0.00	H
ATOM	60	2HG2	VAL	54	104.802	118.112	86.769	1.00	0.00	H
ATOM	61	3HG2	VAL	54	103.964	119.104	85.567	1.00	0.00	H
ATOM	62	1HG2	VAL	54	103.140	118.642	87.079	1.00	0.00	H
ATOM	63	N	ARG	55	101.311	114.102	86.439	0.00	0.00	N
ATOM	64	CA	ARG	55	100.503	113.002	85.830	0.00	0.00	C
ATOM	65	C	ARG	55	99.683	113.480	84.579	0.00	0.00	C
ATOM	66	O	ARG	55	98.913	114.441	84.665	0.00	0.00	O
ATOM	67	CB	ARG	55	99.533	112.395	86.882	0.00	0.00	C
ATOM	68	CG	ARG	55	100.151	111.773	88.159	0.00	0.00	C
ATOM	69	CD	ARG,	55	99.092	111.038	88.997	0.00	0.00	C
ATOM	70	NE	ARG	55	99.641	110.761	90.348	0.00	0.00	N
ATOM	71	CZ	ARG	55	98.978	110.180	91.339	0.00	0.00	C
ATOM	72	NH1	ARG	55	97.772	109.704	91.239	0.00	0.00	N
ATOM	73	NH2	ARG	55	99.572	110.091	92.474	0.00	0.00	N
ATOM	74	HE	ARG	55	100.615	111.041	90.530	1.00	0.00	H
ATOM	75	H	ARG	55	100.954	114.668	87.214	0.00	0.00	H
ATOM	76	HA	ARG	55	101.187	112.185	85.519	0.00	0.00	H
ATOM	77	1HB	ARG	55	98.926	111.617	86.379	0.00	0.00	H
ATOM	78	2HB	ARG	55	98.793	113.166	87.182	0.00	0.00	H
ATOM	79	1HG	ARG	55	100.628	112.570	88.763	0.00	0.00	H
ATOM	80	2HG	ARG	55	100.970	111.072	87.909	0.00	0.00	H
ATOM	81	1HD	ARG	55	98.785	110.098	88.493	0.00	0.00	H
ATOM	82	2HD	ARG	55	98.176	111.658	89.090	0.00	0.00	H
ATOM	83	1HH1	ARG	55	97.371	109.276	92.070	0.00	0.00	H
ATOM	84	2HH1	ARG	55	97.378	109.802	90.301	0.00	0.00	H
ATOM	85	1HH2	ARG	55	99.060	109.677	93.250	0.00	0.00	H
ATOM	86	2HH2	ARG	55	100.498	110.524	92.448	0.00	0.00	H
ATOM	87	N	GLY	56	99.823	112.791	83.436	1.00	0.00	N
ATOM	88	CA	GLY	56	99.062	113.119	82.194	1.00	0.00	C
ATOM	89	C	GLY	56	97.780	112.295	81.942	1.00	0.00	C
ATOM	90	O	GLY	56	96.678	112.843	81.956	1.00	0.00	O
ATOM	91	H	GLY	56	100.528	112.039	83.459	1.00	0.00	H
ATOM	92	1HA	GLY	56	98.786	114.192	82.166	1.00	0.00	H
ATOM	93	2HA	GLY	56	99.729	112.995	81.322	1.00	0.00	H
ATOM	94	N	ARG	57	97.923	110.991	81.655	1.00	0.00	N
ATOM	95	CA	ARG	57	96.765	110.087	81.374	1.00	0.00	C
ATOM	96	C	ARG	57	97.000	108.655	81.967	1.00	0.00	C
ATOM	97	O	ARG	57	98.134	108.174	82.064	1.00	0.00	O
ATOM	98	CB	ARG	57	96.526	110.079	79.834	1.00	0.00	C
ATOM	99	CG	ARG	57	95.213	109.398	79.373	1.00	0.00	C
ATOM	100	CD	ARG	57	94.996	109.479	77.856	1.00	0.00	C
ATOM	101	NE	ARG	57	93.701	108.821	77.548	1.00	0.00	N
ATOM	102	CZ	ARG	57	93.241	108.542	76.337	1.00	0.00	C
ATOM	103	NH1	ARG	57	93.863	108.827	75.232	1.00	0.00	N
ATOM	104	NH2	ARG	57	92.101	107.952	76.262	1.00	0.00	N
ATOM	105	HE	ARG	57	93.108	108.556	78.347	1.00	0.00	H
ATOM	106	H	ARG	57	98.881	110.643	81.765	1.00	0.00	H
ATOM	107	HA	ARG	57	95.857	110.497	81.863	1.00	0.00	H
ATOM	108	1HB	ARG	57	96.511	111.124	79.467	1.00	0.00	H
ATOM	109	2HB	ARG	57	97.390	109.607	79.326	1.00	0.00	H
ATOM	110	1HC	ARG	57	95.204	108.329	79.670	1.00	0.00	H
ATOM	111	2HG	ARG	57	94.345	109.851	79.850	1.00	0.00	H
ATOM	112	1HD	ARG	57	91.901	110.851	77.315	1.00	0.00	H
[illegible]										

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ATOM    124  CD1 PHE    58      92.925 104.888  82.221  1.00  0.00           C
ATOM    125  CE1 PHE    58      91.712 104.847  81.539  1.00  0.00           C
ATOM    126  CZ  PHE    58      90.924 105.992  81.449  1.00  0.00           C
ATOM    127  CE2 PHE    58      91.347 107.179  82.043  1.00  0.00           C
ATOM    128  CD2 PHE    58      92.561 107.221  82.725  1.00  0.00           C
ATOM    129  H   PHE    58      95.026 108.372  82.064  1.00  0.00           H
ATOM    130  HA  PHE    58      96.818 106.419  83.454  1.00  0.00           H
ATOM    131 1HB  PHE    58      94.904 105.145  84.019  1.00  0.00           H
ATOM    132 2HB  PHE    58      94.636 106.807  84.415  1.00  0.00           H
ATOM    133  HD1 PHE    58      93.540 103.999  82.262  1.00  0.00           H
ATOM    134  HE1 PHE    58      91.388 103.929  81.068  1.00  0.00           H
ATOM    135  HZ  PHE    58      89.986 105.961  80.913  1.00  0.00           H
ATOM    136  HE2 PHE    58      90.738 108.067  81.966  1.00  0.00           H
ATOM    137  HD2 PHE    58      92.882 108.149  83.179  1.00  0.00           H
ATOM    138  N   LEU    59      97.255 104.662  81.698  0.00  0.00           N
ATOM    139  CA  LEU    59      97.536 103.546  80.752  0.00  0.00           C
ATOM    140  C   LEU    59      96.581 102.327  81.038  0.00  0.00           C
ATOM    141  O   LEU    59      95.715 102.031  80.211  0.00  0.00           O
ATOM    142  CB  LEU    59      99.079 103.309  80.853  0.00  0.00           C
ATOM    143  CG  LEU    59      99.808 102.416  79.817  0.00  0.00           C
ATOM    144  CD1 LEU    59      99.468 100.925  79.926  0.00  0.00           C
ATOM    145  CD2 LEU    59      99.633 102.897  78.369  0.00  0.00           C
ATOM    146  H   LEU    59      97.696 104.671  82.627  0.00  0.00           H
ATOM    147  HA  LEU    59      97.324 103.877  79.716  0.00  0.00           H
ATOM    148 1HB  LEU    59      99.334 102.939  81.865  0.00  0.00           H
ATOM    149 2HB  LEU    59      99.594 104.291  80.798  0.00  0.00           H
ATOM    150  HG  LEU    59     100.892 102.501  80.047  0.00  0.00           H
ATOM    151 1HD1 LEU    59      99.582 100.542  80.956  0.00  0.00           H
ATOM    152 2HD1 LEU    59      98.436 100.688  79.606  0.00  0.00           H
ATOM    153 3HD1 LEU    59     100.153 100.321  79.304  0.00  0.00           H
ATOM    154 1HD2 LEU    59     100.279 102.327  77.675  0.00  0.00           H
ATOM    155 2HD2 LEU    59      98.592 102.786  78.012  0.00  0.00           H
ATOM    156 3HD2 LEU    59      99.915 103.961  78.256  0.00  0.00           H
ATOM    157  N   GLY    60      96.676 101.691  82.223  0.00  0.00           N
ATOM    158  CA  GLY    60      95.847 100.505  82.595  0.00  0.00           C
ATOM    159  C   GLY    60      95.373 100.470  84.075  0.00  0.00           C
ATOM    160  O   GLY    60      95.769 101.287  84.920  0.00  0.00           O
ATOM    161  H   GLY    60      97.447 102.031  82.805  0.00  0.00           H
ATOM    162 1HA  GLY    60      96.432  99.582  82.395  0.00  0.00           H
ATOM    163 2HA  GLY    60      94.967 100.400  81.931  0.00  0.00           H
ATOM    164  N   LYS    61      94.466  99.529  84.393  1.00  0.00           N
ATOM    165  CA  LYS    61      93.868  99.405  85.758  1.00  0.00           C
ATOM    166  C   LYS    61      93.299  97.972  86.042  1.00  0.00           C
ATOM    167  O   LYS    61      92.266  97.584  85.486  1.00  0.00           O
ATOM    168  CB  LYS    61      92.744 100.472  85.958  1.00  0.00           C
ATOM    169  CG  LYS    61      92.217 100.597  87.406  1.00  0.00           C
ATOM    170  CD  LYS    61      91.152 101.703  87.529  1.00  0.00           C
ATOM    171  CE  LYS    61      90.610 101.830  88.958  1.00  0.00           C
ATOM    172  NZ  LYS    61      89.603 102.910  89.003  1.00  0.00           N
ATOM    173 1HZ  LYS    61      89.236 102.999  89.961  1.00  0.00           H
ATOM    174 2HZ  LYS    61      90.040 103.799  88.719  1.00  0.00           H
ATOM    175 3HZ  LYS    61      88.831 102.687  88.359  1.00  0.00           H
ATOM    176  H   LYS    61      94.523  98.723  83.745  1.00  0.00           H
ATOM    177  HA  LYS    61      94.668  99.606  86.500  1.00  0.00           H
ATOM    178 1HB  LYS    61      93.112 101.471  85.646  1.00  0.00           H
ATOM    179 2HB  LYS    61      91.900 100.252  85.275  1.00  0.00           H
ATOM    180 1HG  LYS    61      91.791  99.629  87.739  1.00  0.00           H
ATOM    181 2HG  LYS    61      93.058 100.804  88.098  1.00  0.00           H
ATOM    182 1HD  LYS    61      91.583 102.672  87.205  1.00  0.00           H
ATOM    183 2HD  LYS    61      90.322 101.497  86.825  1.00  0.00           H
ATOM    184 1HE  LYS    61      90.160 100.873  89.292  1.00  0.00           H
ATOM    185 2HE  LYS    61      91.431 102.052  89.669  1.00  0.00           H
ATOM    186  N   GLY    62      93.868  97.257  87.026  0.00  0.00           N
ATOM    187  CA  GLY    62      93.338  95.929  87.443  0.00  0.00           C
ATOM    188  C   GLY    62      93.782  95.448  88.844  0.00  0.00           C
ATOM    189  O   GLY    62      93.881  96.219  89.801  0.00  0.00           O
ATOM    190  H   GLY    62      94.799  97.595  87.296  0.00  0.00           H
ATOM    191 1HA  GLY    62      93.630  95.190  86.668  0.00  0.00           H
ATOM    192 2HA  GLY    62      92.228  95.918  87.437  0.00  0.00           H
ATOM    193  N   GLY    63      94.055  94.138  88.968  1.00  0.00           N
ATOM    194  CA  GLY    63      94.411  93.510  90.288  1.00  0.00           C
ATOM    195  C   GLY    63      95.817  93.707  90.924  1.00  0.00           C
ATOM    196  O   GLY    63      96.231  92.889  91.746  1.00  0.00           O
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ATOM	197	H	GLY	63	93.953	93.598	88.103	1.00	0.00	H
ATOM	198	1HA	GLY	63	93.677	93.819	91.056	1.00	0.00	H
ATOM	199	2HA	GLY	63	94.259	92.418	90.203	1.00	0.00	H
ATOM	200	N	PHE	64	96.503	94.806	90.594	0.00	0.00	N
ATOM	201	CA	PHE	64	97.650	95.340	91.383	0.00	0.00	C
ATOM	202	C	PHE	64	97.219	96.766	91.673	0.00	0.00	C
ATOM	203	O	PHE	64	96.780	96.906	93.017	0.00	0.00	O
ATOM	204	CB	PHE	64	98.957	95.211	90.531	0.00	0.00	C
ATOM	205	CG	PHE	64	100.322	95.180	91.262	0.00	0.00	C
ATOM	206	CD1	PHE	64	101.339	94.374	90.729	0.00	0.00	C
ATOM	207	CE1	PHE	64	102.589	94.313	91.339	0.00	0.00	C
ATOM	208	CZ	PHE	64	102.844	95.070	92.476	0.00	0.00	C
ATOM	209	CE2	PHE	64	101.849	95.880	93.015	0.00	0.00	C
ATOM	210	CD2	PHE	64	100.597	95.943	92.407	0.00	0.00	C
ATOM	211	H	PHE	64	96.013	95.366	89.888	0.00	0.00	H
ATOM	212	HA	PHE	64	97.815	94.744	92.306	0.00	0.00	H
ATOM	213	1HB	PHE	64	98.995	95.988	89.745	0.00	0.00	H
ATOM	214	2HB	PHE	64	98.885	94.272	89.943	0.00	0.00	H
ATOM	215	HD1	PHE	64	101.175	93.786	89.834	0.00	0.00	H
ATOM	216	HE1	PHE	64	103.371	93.687	90.923	0.00	0.00	H
ATOM	217	HZ	PHE	64	103.822	95.022	92.935	0.00	0.00	H
ATOM	218	HE2	PHE	64	102.058	96.458	93.903	0.00	0.00	H
ATOM	219	HD2	PHE	64	99.845	96.585	92.839	0.00	0.00	H
ATOM	220	N	ALA	65	97.243	97.795	90.990	1.00	0.00	N
ATOM	221	CA	ALA	65	96.401	99.013	91.144	1.00	0.00	C
ATOM	222	C	ALA	65	96.155	99.807	89.814	1.00	0.00	C
ATOM	223	O	ALA	65	95.088	99.660	89.208	1.00	0.00	O
ATOM	224	CB	ALA	65	96.915	99.890	92.311	1.00	0.00	C
ATOM	225	H	ALA	65	97.644	97.519	90.086	1.00	0.00	H
ATOM	226	HA	ALA	65	95.375	98.686	91.416	1.00	0.00	H
ATOM	227	2HB	ALA	65	96.805	99.369	93.278	1.00	0.00	H
ATOM	228	3HB	ALA	65	97.986	100.139	92.197	1.00	0.00	H
ATOM	229	1HB	ALA	65	96.357	100.841	92.391	1.00	0.00	H
ATOM	230	N	LYS	66	97.056	100.720	89.405	1.00	0.00	N
ATOM	231	CA	LYS	66	96.846	101.620	88.233	1.00	0.00	C
ATOM	232	C	LYS	66	98.200	102.188	87.702	1.00	0.00	C
ATOM	233	O	LYS	66	98.947	102.808	88.469	1.00	0.00	O
ATOM	234	CB	LYS	66	95.815	102.752	88.564	1.00	0.00	C
ATOM	235	CG	LYS	66	96.230	103.839	89.590	1.00	0.00	C
ATOM	236	CD	LYS	66	95.060	104.754	89.991	1.00	0.00	C
ATOM	237	CE	LYS	66	95.529	105.928	90.862	1.00	0.00	C
ATOM	238	NZ	LYS	66	94.373	106.785	91.189	1.00	0.00	N
ATOM	239	1HZ	LYS	66	94.684	107.574	91.773	1.00	0.00	H
ATOM	240	2HZ	LYS	66	93.956	107.146	90.319	1.00	0.00	H
ATOM	241	3HZ	LYS	66	93.670	106.234	91.702	1.00	0.00	H
ATOM	242	H	LYS	66	97.952	100.685	89.906	1.00	0.00	H
ATOM	243	HA	LYS	66	96.407	101.006	87.418	1.00	0.00	H
ATOM	244	1HB	LYS	66	95.539	103.250	87.615	1.00	0.00	H
ATOM	245	2HB	LYS	66	94.875	102.272	88.900	1.00	0.00	H
ATOM	246	1HG	LYS	66	96.657	103.368	90.497	1.00	0.00	H
ATOM	247	2HG	LYS	66	97.055	104.444	89.163	1.00	0.00	H
ATOM	248	1HD	LYS	66	94.549	105.136	89.086	1.00	0.00	H
ATOM	249	2HD	LYS	66	94.294	104.158	90.526	1.00	0.00	H
ATOM	250	1HE	LYS	66	96.013	105.558	91.789	1.00	0.00	H
ATOM	251	2HE	LYS	66	96.299	106.524	90.330	1.00	0.00	H
ATOM	252	N	CYS	67	98.478	102.033	86.400	1.00	0.00	N
ATOM	253	CA	CYS	67	99.654	102.670	85.746	1.00	0.00	C
ATOM	254	C	CYS	67	99.278	103.971	84.964	1.00	0.00	C
ATOM	255	O	CYS	67	98.198	104.091	84.372	1.00	0.00	O
ATOM	256	CB	CYS	67	100.379	101.592	84.922	1.00	0.00	C
ATOM	257	SG	CYS	67	99.311	100.811	83.659	1.00	0.00	S
ATOM	258	H	CYS	67	97.759	101.361	85.822	1.00	0.00	H

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ATOM    270  CE1 PHE    68      96.435 109.246  85.843  1.00  0.00           C
ATOM    271  CZ  PHE    68      95.682 108.371  86.620  1.00  0.00           C
ATOM    272  CE2 PHE    68      96.228 107.159  87.035  1.00  0.00           C
ATOM    273  CD2 PHE    68      97.532 106.823  86.682  1.00  0.00           C
ATOM    274  H   PHE    68     101.038 104.758  85.528  1.00  0.00           H
ATOM    275  HA  PHE    68      99.054 106.312  83.764  1.00  0.00           H
ATOM    276 1HB  PHE    68     100.300 107.066  86.470  1.00  0.00           H
ATOM    277 2HB  PHE    68     100.257 108.312  85.283  1.00  0.00           H
ATOM    278  HD1 PHE    68      98.312 109.598  84.877  1.00  0.00           H
ATOM    279  HE1 PHE    68      96.009 110.183  85.512  1.00  0.00           H
ATOM    280  HZ  PHE    68      94.669 108.628  86.896  1.00  0.00           H
ATOM    281  HE2 PHE    68      95.640 106.480  87.633  1.00  0.00           H
ATOM    282  HD2 PHE    68      97.947 105.882  87.013  1.00  0.00           H
ATOM    283  N   GLU    69     100.875 107.502  82.456  1.00  0.00           N
ATOM    284  CA  GLU    69     101.904 108.317  81.744  1.00  0.00           C
ATOM    285  C   GLU    69     102.269 109.587  82.591  1.00  0.00           C
ATOM    286  O   GLU    69     101.475 110.527  82.695  1.00  0.00           O
ATOM    287  CB  GLU    69     101.313 108.631  80.346  1.00  0.00           C
ATOM    288  CG  GLU    69     102.257 109.425  79.404  1.00  0.00           C
ATOM    289  CD  GLU    69     101.724 109.581  77.983  1.00  0.00           C
ATOM    290  OE1 GLU    69     101.463 108.612  77.239  1.00  0.00           O
ATOM    291  OE2 GLU    69     101.433 110.872  77.674  1.00  0.00           O
ATOM    292  H   GLU    69      99.870 107.688  82.316  1.00  0.00           H
ATOM    293  HA  GLU    69     102.816 107.705  81.581  1.00  0.00           H
ATOM    294 1HB  GLU    69     101.047 107.679  79.841  1.00  0.00           H
ATOM    295 2HB  GLU    69     100.356 109.179  80.447  1.00  0.00           H
ATOM    296 1HG  GLU    69     102.471 110.425  79.828  1.00  0.00           H
ATOM    297 2HG  GLU    69     103.236 108.929  79.306  1.00  0.00           H
ATOM    298  N   ILE    70     103.448 109.579  83.229  1.00  0.00           N
ATOM    299  CA  ILE    70     103.873 110.642  84.193  1.00  0.00           C
ATOM    300  C   ILE    70     105.179 111.309  83.637  1.00  0.00           C
ATOM    301  O   ILE    70     106.208 110.650  83.454  1.00  0.00           O
ATOM    302  CB  ILE    70     104.059 110.093  85.662  1.00  0.00           C
ATOM    303  CG1 ILE    70     102.877 109.225  86.195  1.00  0.00           C
ATOM    304  CG2 ILE    70     104.317 111.255  86.658  1.00  0.00           C
ATOM    305  CD1 ILE    70     103.026 108.633  87.611  1.00  0.00           C
ATOM    306  H   ILE    70     103.997 108.715  83.099  1.00  0.00           H
ATOM    307  HA  ILE    70     103.089 111.422  84.256  1.00  0.00           H
ATOM    308  HB  ILE    70     104.960 109.444  85.657  1.00  0.00           H
ATOM    309 1HG1 ILE    70     101.931 109.795  86.130  1.00  0.00           H
ATOM    310 2HG1 ILE    70     102.737 108.371  85.507  1.00  0.00           H
ATOM    311 2HG2 ILE    70     105.106 111.947  86.313  1.00  0.00           H
ATOM    312 3HG2 ILE    70     103.412 111.865  86.831  1.00  0.00           H
ATOM    313 1HG2 ILE    70     104.649 110.880  87.643  1.00  0.00           H
ATOM    314 2HD1 ILE    70     104.015 108.167  87.762  1.00  0.00           H
ATOM    315 3HD1 ILE    70     102.906 109.405  88.395  1.00  0.00           H
ATOM    316 1HD1 ILE    70     102.263 107.858  87.810  1.00  0.00           H
ATOM    317  N   SER    71     105.152 112.631  83.413  1.00  0.00           N
ATOM    318  CA  SER    71     106.376 113.412  83.098  1.00  0.00           C
ATOM    319  C   SER    71     107.154 113.834  84.385  1.00  0.00           C
ATOM    320  O   SER    71     106.586 114.421  85.309  1.00  0.00           O
ATOM    321  CB  SER    71     105.960 114.645  82.265  1.00  0.00           C
ATOM    322  OG  SER    71     107.110 115.366  81.807  1.00  0.00           O
ATOM    323  H   SER    71     104.293 113.093  83.746  1.00  0.00           H
ATOM    324  HA  SER    71     107.043 112.810  82.450  1.00  0.00           H
ATOM    325 1HB  SER    71     105.366 114.332  81.383  1.00  0.00           H
ATOM    326 2HB  SER    71     105.297 115.316  82.847  1.00  0.00           H
ATOM    327  HG  SER    71     107.585 115.699  82.578  1.00  0.00           H
ATOM    328  N   ASP    72     108.478 113.631  84.406  1.00  0.00           N
ATOM    329  CA  ASP    72     109.394 114.350  85.338  1.00  0.00           C
ATOM    330  C   ASP    72     109.438 115.878  84.976  1.00  0.00           C
ATOM    331  O   ASP    72     109.784 116.245  83.851  1.00  0.00           O
ATOM    332  CB  ASP    72     110.803 113.684  85.270  1.00  0.00           C
ATOM    333  CG  ASP    72     111.439 113.276  86.597  1.00  0.00           C
ATOM    334  OD1 ASP    72     111.932 112.171  86.785  1.00  0.00           O
ATOM    335  OD2 ASP    72     111.409 114.257  87.539  1.00  0.00           O
ATOM    336  H   ASP    72     108.829 113.054  83.626  1.00  0.00           H
ATOM    337  HA  ASP    72     108.993 114.230  86.367  1.00  0.00           H
ATOM    338 1HB  ASP    72     110.779 112.765  84.660  1.00  0.00           H
ATOM    339 2HB  ASP    72     111.527 114.326  84.736  1.00  0.00           H
ATOM    340  N   ALA    73     109.010 116.750  85.893  1.00  0.00           N
ATOM    341  CA  ALA    73     108.809 118.199  85.618  1.00  0.00           C
ATOM    342  C   ALA    73     110.090 119.067  85.378  1.00  0.00           C
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ATOM    343  O   ALA    73     110.112 119.894  84.466  1.00  0.00           O
ATOM    344  CB  ALA    73     107.957 118.712  86.796  1.00  0.00           C
ATOM    345  H   ALA    73     108.846 116.340  86.825  1.00  0.00           H
ATOM    346  HA  ALA    73     108.197 118.298  84.699  1.00  0.00           H
ATOM    347 2HB  ALA    73     107.046 118.105  86.956  1.00  0.00           H
ATOM    348 3HB  ALA    73     108.520 118.720  87.749  1.00  0.00           H
ATOM    349 1HB  ALA    73     107.622 119.748  86.618  1.00  0.00           H
ATOM    350  N   ASP    74     111.144 118.878  86.187  1.00  0.00           N
ATOM    351  CA  ASP    74     112.426 119.637  86.060  1.00  0.00           C
ATOM    352  C   ASP    74     113.439 119.098  84.983  1.00  0.00           C
ATOM    353  O   ASP    74     114.168 119.901  84.399  1.00  0.00           O
ATOM    354  CB  ASP    74     113.039 119.767  87.483  1.00  0.00           C
ATOM    355  CG  ASP    74     112.259 120.707  88.409  1.00  0.00           C
ATOM    356  OD1 ASP    74     112.543 121.888  88.568  1.00  0.00           O
ATOM    357  OD2 ASP    74     111.176 120.106  88.975  1.00  0.00           O
ATOM    358  H   ASP    74     110.954 118.227  86.954  1.00  0.00           H
ATOM    359  HA  ASP    74     112.196 120.667  85.713  1.00  0.00           H
ATOM    360 1HB  ASP    74     113.155 118.780  87.967  1.00  0.00           H
ATOM    361 2HB  ASP    74     114.063 120.175  87.408  1.00  0.00           H
ATOM    362  N   THR    75     113.491 117.782  84.701  0.00  0.00           N
ATOM    363  CA  THR    75     114.274 117.208  83.552  0.00  0.00           C
ATOM    364  C   THR    75     113.505 117.002  82.190  0.00  0.00           C
ATOM    365  O   THR    75     114.162 116.797  81.167  0.00  0.00           O
ATOM    366  CB  THR    75     114.958 115.866  83.972  0.00  0.00           C
ATOM    367  OG1 THR    75     114.001 114.890  84.377  0.00  0.00           O
ATOM    368  CG2 THR    75     116.000 115.964  85.096  0.00  0.00           C
ATOM    369  H   THR    75     112.860 117.204  85.264  0.00  0.00           H
ATOM    370  HA  THR    75     115.099 117.901  83.291  0.00  0.00           H
ATOM    371  HB  THR    75     115.494 115.471  83.084  0.00  0.00           H
ATOM    372  HG1 THR    75     114.468 114.041  84.362  0.00  0.00           H
ATOM    373 1HG2 THR    75     116.485 114.990  85.288  0.00  0.00           H
ATOM    374 2HG2 THR    75     116.800 116.685  84.847  0.00  0.00           H
ATOM    375 3HG2 THR    75     115.544 116.296  86.048  0.00  0.00           H
ATOM    376  N   LYS    76     112.156 117.002  82.157  1.00  0.00           N
ATOM    377  CA  LYS    76     111.326 116.626  80.966  1.00  0.00           C
ATOM    378  C   LYS    76     111.521 115.147  80.454  1.00  0.00           C
ATOM    379  O   LYS    76     111.955 114.899  79.326  1.00  0.00           O
ATOM    380  CB  LYS    76     111.377 117.750  79.890  1.00  0.00           C
ATOM    381  CG  LYS    76     110.215 117.715  78.869  1.00  0.00           C
ATOM    382  CD  LYS    76     110.269 118.893  77.878  1.00  0.00           C
ATOM    383  CE  LYS    76     109.083 118.874  76.902  1.00  0.00           C
ATOM    384  NZ  LYS    76     109.178 120.032  75.991  1.00  0.00           N
ATOM    385 1HZ  LYS    76     108.383 120.020  75.336  1.00  0.00           H
ATOM    386 2HZ  LYS    76     109.156 120.904  76.540  1.00  0.00           H
ATOM    387 3HZ  LYS    76     110.059 119.982  75.461  1.00  0.00           H
ATOM    388  H   LYS    76     111.732 117.241  83.060  1.00  0.00           H
ATOM    389  HA  LYS    76     110.283 116.647  81.335  1.00  0.00           H
ATOM    390 1HB  LYS    76     111.373 118.738  80.390  1.00  0.00           H
ATOM    391 2HB  LYS    76     112.350 117.701  79.362  1.00  0.00           H
ATOM    392 1HG  LYS    76     110.236 116.758  78.310  1.00  0.00           H
ATOM    393 2HG  LYS    76     109.246 117.726  79.405  1.00  0.00           H
ATOM    394 1HD  LYS    76     110.276 119.850  78.439  1.00  0.00           H
ATOM    395 2HD  LYS    76     111.226 118.866  77.323  1.00  0.00           H
ATOM    396 1HE  LYS    76     109.072 117.929  76.323  1.00  0.00           H
ATOM    397 2HE  LYS    76     108.124 118.910  77.455  1.00  0.00           H
ATOM    398  N   GLU    77     111.182 114.160  81.304  1.00  0.00           N
ATOM    399  CA  GLU    77     111.388 112.710  81.010  1.00  0.00           C
ATOM    400  C   GLU    77     110.056 111.924  81.242  1.00  0.00           C
ATOM    401  O   GLU    77     109.498 111.953  82.341  1.00  0.00           O
ATOM    402  CB  GLU    77     112.526 112.150  81.907  1.00  0.00           C
ATOM    403  CG  GLU    77     113.952 112.697  81.620  1.00  0.00           C
ATOM    404  CD  GLU    77     115.003 112.121  82.539  1.00  0.00           C
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ATOM    416  O   VAL    78     109.020 108.243  80.129  1.00  0.00           O
ATOM    417  CB  VAL    78     107.372 110.787  78.964  1.00  0.00           C
ATOM    418  CG1 VAL    78     106.959 112.261  78.749  1.00  0.00           C
ATOM    419  CG2 VAL    78     108.015 110.259  77.661  1.00  0.00           C
ATOM    420  H   VAL    78     110.071 111.278  79.345  1.00  0.00           H
ATOM    421  HA  VAL    78     107.598 111.065  81.062  1.00  0.00           H
ATOM    422  HB  VAL    78     106.424 110.234  79.103  1.00  0.00           H
ATOM    423 1HG1 VAL    78     107.833 112.918  78.578  1.00  0.00           H
ATOM    424 2HG1 VAL    78     106.287 112.382  77.879  1.00  0.00           H
ATOM    425 3HG1 VAL    78     106.421 112.669  79.625  1.00  0.00           H
ATOM    426 2HG2 VAL    78     108.267 109.184  77.736  1.00  0.00           H
ATOM    427 3HG2 VAL    78     107.338 110.363  76.794  1.00  0.00           H
ATOM    428 1HG2 VAL    78     108.950 110.791  77.408  1.00  0.00           H
ATOM    429  N   PHE    79     107.458 108.656  81.701  1.00  0.00           N
ATOM    430  CA  PHE    79     107.559 107.335  82.387  1.00  0.00           C
ATOM    431  C   PHE    79     106.160 106.654  82.583  1.00  0.00           C
ATOM    432  O   PHE    79     105.163 107.290  82.943  1.00  0.00           O
ATOM    433  CB  PHE    79     108.193 107.551  83.793  1.00  0.00           C
ATOM    434  CG  PHE    79     109.667 107.986  83.837  1.00  0.00           C
ATOM    435  CD1 PHE    79     110.007 109.280  84.244  1.00  0.00           C
ATOM    436  CE1 PHE    79     111.344 109.666  84.309  1.00  0.00           C
ATOM    437  CZ  PHE    79     112.347 108.773  83.948  1.00  0.00           C
ATOM    438  CE2 PHE    79     112.018 107.481  83.544  1.00  0.00           C
ATOM    439  CD2 PHE    79     110.684 107.088  83.496  1.00  0.00           C
ATOM    440  H   PHE    79     106.996 109.437  82.183  1.00  0.00           H
ATOM    441  HA  PHE    79     108.209 106.643  81.810  1.00  0.00           H
ATOM    442 1HB  PHE    79     107.558 108.258  84.363  1.00  0.00           H
ATOM    443 2HB  PHE    79     108.124 106.607  84.368  1.00  0.00           H
ATOM    444  HD1 PHE    79     109.236 109.992  84.503  1.00  0.00           H
ATOM    445  HE1 PHE    79     111.609 110.656  84.642  1.00  0.00           H
ATOM    446  HZ  PHE    79     113.384 109.073  84.006  1.00  0.00           H
ATOM    447  HE2 PHE    79     112.798 106.782  83.282  1.00  0.00           H
ATOM    448  HD2 PHE    79     110.445 106.085  83.177  1.00  0.00           H
ATOM    449  N   ALA    80     106.110 105.319  82.471  0.00  0.00           N
ATOM    450  CA  ALA    80     104.990 104.508  83.001  0.00  0.00           C
ATOM    451  C   ALA    80     105.107 104.272  84.547  0.00  0.00           C
ATOM    452  O   ALA    80     105.868 103.428  85.035  0.00  0.00           O
ATOM    453  CB  ALA    80     105.012 103.194  82.218  0.00  0.00           C
ATOM    454  H   ALA    80     107.042 104.891  82.358  0.00  0.00           H
ATOM    455  HA  ALA    80     104.026 105.000  82.765  0.00  0.00           H
ATOM    456 1HB  ALA    80     104.222 102.506  82.564  0.00  0.00           H
ATOM    457 2HB  ALA    80     104.850 103.354  81.136  0.00  0.00           H
ATOM    458 3HB  ALA    80     105.975 102.656  82.325  0.00  0.00           H
ATOM    459  N   GLY    81     104.345 105.047  85.329  1.00  0.00           N
ATOM    460  CA  GLY    81     104.419 105.001  86.811  1.00  0.00           C
ATOM    461  C   GLY    81     103.218 104.300  87.487  1.00  0.00           C
ATOM    462  O   GLY    81     102.070 104.747  87.385  1.00  0.00           O
ATOM    463  H   GLY    81     103.838 105.767  84.788  1.00  0.00           H
ATOM    464 1HA  GLY    81     105.375 104.556  87.150  1.00  0.00           H
ATOM    465 2HA  GLY    81     104.492 106.029  87.189  1.00  0.00           H
ATOM    466  N   LYS    82     103.500 103.207  88.205  0.00  0.00           N
ATOM    467  CA  LYS    82     102.483 102.410  88.951  0.00  0.00           C
ATOM    468  C   LYS    82     102.243 102.984  90.404  0.00  0.00           C
ATOM    469  O   LYS    82     103.163 102.982  91.231  0.00  0.00           O
ATOM    470  CB  LYS    82     102.939 100.916  88.804  0.00  0.00           C
ATOM    471  CG  LYS    82     102.310  99.855  89.746  0.00  0.00           C
ATOM    472  CD  LYS    82     102.506  98.366  89.344  0.00  0.00           C
ATOM    473  CE  LYS    82     103.964  97.854  89.290  0.00  0.00           C
ATOM    474  NZ  LYS    82     104.023  96.406  88.932  0.00  0.00           N
ATOM    475 1HZ  LYS    82     103.258  95.811  89.258  1.00  0.00           H
ATOM    476 2HZ  LYS    82     104.049  96.196  87.906  1.00  0.00           H
ATOM    477 3HZ  LYS    82     104.877  95.915  89.296  1.00  0.00           H
ATOM    478  H   LYS    82     104.503 102.956  88.189  0.00  0.00           H
ATOM    479  HA  LYS    82     101.518 102.463  88.412  0.00  0.00           H
ATOM    480 1HB  LYS    82     104.038 100.839  88.899  0.00  0.00           H
ATOM    481 2HB  LYS    82     102.760 100.609  87.752  0.00  0.00           H
ATOM    482 1HG  LYS    82     101.223 100.047  89.831  0.00  0.00           H
ATOM    483 2HG  LYS    82     102.711 100.010  90.766  0.00  0.00           H
ATOM    484 1HD  LYS    82     102.006  98.183  88.371  0.00  0.00           H
ATOM    485 2HD  LYS    82     101.939  97.735  90.057  0.00  0.00           H
ATOM    486 1HE  LYS    82     104.477  98.016  90.265  0.00  0.00           H
ATOM    487 2HE  LYS    82     104.562  98.441  88.556  0.00  0.00           H
ATOM    488  N   ILE    83     101.013 103.425  90.715  0.00  0.00           N
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ATOM	489	CA	ILE	83	100.653	103.996	92.050	0.00	0.00	C
ATOM	490	C	ILE	83	99.997	102.861	92.910	0.00	0.00	C
ATOM	491	O	ILE	83	98.864	102.450	92.636	0.00	0.00	O
ATOM	492	CB	ILE	83	99.731	105.267	91.908	0.00	0.00	C
ATOM	493	CG2	ILE	83	99.435	105.908	93.291	0.00	0.00	C
ATOM	494	CG1	ILE	83	100.274	106.395	90.972	0.00	0.00	C
ATOM	495	CD1	ILE	83	99.796	106.303	89.513	0.00	0.00	C
ATOM	496	H	ILE	83	100.334	103.382	89.944	0.00	0.00	H
ATOM	497	HA	ILE	83	101.573	104.343	92.566	0.00	0.00	H
ATOM	498	HB	ILE	83	98.753	104.929	91.502	0.00	0.00	H
ATOM	499	1HG2	ILE	83	98.747	106.771	93.207	0.00	0.00	H
ATOM	500	2HG2	ILE	83	98.949	105.197	93.985	0.00	0.00	H
ATOM	501	3HG2	ILE	83	100.356	106.268	93.788	0.00	0.00	H
ATOM	502	1HG1	ILE	83	101.381	106.416	91.000	0.00	0.00	H
ATOM	503	2HG1	ILE	83	99.975	107.399	91.330	0.00	0.00	H
ATOM	504	1HD1	ILE	83	100.166	107.159	88.919	0.00	0.00	H
ATOM	505	2HD1	ILE	83	100.143	105.386	89.003	0.00	0.00	H
ATOM	506	3HD1	ILE	83	98.693	106.323	89.443	0.00	0.00	H
ATOM	507	N	VAL	84	100.698	102.366	93.944	1.00	0.00	N
ATOM	508	CA	VAL	84	100.244	101.190	94.755	1.00	0.00	C
ATOM	509	C	VAL	84	99.727	101.685	96.168	1.00	0.00	C
ATOM	510	O	VAL	84	100.568	101.985	97.027	1.00	0.00	O
ATOM	511	CB	VAL	84	101.388	100.119	94.872	1.00	0.00	C
ATOM	512	CG1	VAL	84	100.985	98.872	95.691	1.00	0.00	C
ATOM	513	CG2	VAL	84	101.915	99.594	93.519	1.00	0.00	C
ATOM	514	H	VAL	84	101.673	102.693	93.997	1.00	0.00	H
ATOM	515	HA	VAL	84	99.421	100.666	94.236	1.00	0.00	H
ATOM	516	HB	VAL	84	102.238	100.600	95.394	1.00	0.00	H
ATOM	517	1HG1	VAL	84	100.133	98.329	95.239	1.00	0.00	H
ATOM	518	2HG1	VAL	84	101.820	98.152	95.783	1.00	0.00	H
ATOM	519	3HG1	VAL	84	100.689	99.129	96.724	1.00	0.00	H
ATOM	520	2HG2	VAL	84	102.366	100.415	92.933	1.00	0.00	H
ATOM	521	3HG2	VAL	84	102.707	98.831	93.635	1.00	0.00	H
ATOM	522	1HG2	VAL	84	101.112	99.150	92.899	1.00	0.00	H
ATOM	523	N	PRO	85	98.394	101.783	96.473	1.00	0.00	N
ATOM	524	CA	PRO	85	97.898	102.296	97.780	1.00	0.00	C
ATOM	525	C	PRO	85	97.963	101.264	98.958	1.00	0.00	C
ATOM	526	O	PRO	85	97.609	100.091	98.822	1.00	0.00	O
ATOM	527	CB	PRO	85	96.465	102.731	97.410	1.00	0.00	C
ATOM	528	CG	PRO	85	96.034	101.769	96.303	1.00	0.00	C
ATOM	529	CD	PRO	85	97.312	101.509	95.509	1.00	0.00	C
ATOM	530	HA	PRO	85	98.468	103.206	98.052	1.00	0.00	H
ATOM	531	1HB	PRO	85	95.769	102.729	98.270	1.00	0.00	H
ATOM	532	2HB	PRO	85	96.477	103.769	97.020	1.00	0.00	H
ATOM	533	1HG	PRO	85	95.682	100.819	96.743	1.00	0.00	H
ATOM	534	2HG	PRO	85	95.213	102.164	95.675	1.00	0.00	H
ATOM	535	1HD	PRO	85	97.341	100.464	95.147	1.00	0.00	H
ATOM	536	2HD	PRO	85	97.377	102.183	94.633	1.00	0.00	H
ATOM	537	N	LYS	86	98.387	101.742	100.135	0.00	0.00	N
ATOM	538	CA	LYS	86	98.662	100.888	101.331	0.00	0.00	C
ATOM	539	C	LYS	86	97.517	99.968	101.889	0.00	0.00	C
ATOM	540	O	LYS	86	97.759	98.781	102.113	0.00	0.00	O
ATOM	541	CB	LYS	86	99.331	101.795	102.404	0.00	0.00	C
ATOM	542	CG	LYS	86	98.485	102.960	102.985	0.00	0.00	C
ATOM	543	CD	LYS	86	99.335	103.922	103.828	0.00	0.00	C
ATOM	544	CE	LYS	86	98.550	105.160	104.284	0.00	0.00	C
ATOM	545	NZ	LYS	86	99.460	106.049	105.030	0.00	0.00	N
ATOM	546	1HZ	LYS	86	98.944	106.885	105.341	1.00	0.00	H
ATOM	547	2HZ	LYS	86	99.222	105.550	105.951	1.00	0.00	H
ATOM	548	3HZ	LYS	86	100.239	106.335	104.420	1.00	0.00	H
ATOM	549	H	LYS	86	98.689	102.718	100.099	0.00	0.00	H
ATOM	550	[illegible]	LYS	86	98.50	100.171	101.022	0.00	1.00	H

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ATOM    562  O   SER    87      94.403  97.411 101.905  1.00  0.00           O
ATOM    563  CB  SER    87      94.007 100.572 103.026  1.00  0.00           C
ATOM    564  OG  SER    87      92.956  99.832 103.653  1.00  0.00           O
ATOM    565  H   SER    87      96.215 101.475 101.887  1.00  0.00           H
ATOM    566  HA  SER    87      95.461  99.059 103.431  1.00  0.00           H
ATOM    567 1HB  SER    87      94.402 101.305 103.758  1.00  0.00           H
ATOM    568 2HB  SER    87      93.596 101.174 102.191  1.00  0.00           H
ATOM    569  HG  SER    87      92.584  99.229 102.998  1.00  0.00           H
ATOM    570  N   LEU    88      94.447  98.902 100.227  1.00  0.00           N
ATOM    571  CA  LEU    88      94.175  97.890  99.154  1.00  0.00           C
ATOM    572  C   LEU    88      95.362  96.936  98.752  1.00  0.00           C
ATOM    573  O   LEU    88      95.100  95.892  98.156  1.00  0.00           O
ATOM    574  CB  LEU    88      93.567  98.609  97.916  1.00  0.00           C
ATOM    575  CG  LEU    88      92.166  99.261  98.079  1.00  0.00           C
ATOM    576  CD1 LEU    88      91.833 100.106  96.839  1.00  0.00           C
ATOM    577  CD2 LEU    88      91.053  98.218  98.282  1.00  0.00           C
ATOM    578  H   LEU    88      94.777  99.847 100.006  1.00  0.00           H
ATOM    579  HA  LEU    88      93.404  97.191  99.529  1.00  0.00           H
ATOM    580 1HB  LEU    88      94.292  99.365  97.570  1.00  0.00           H
ATOM    581 2HB  LEU    88      93.512  97.889  97.075  1.00  0.00           H
ATOM    582  HG  LEU    88      92.179  99.938  98.956  1.00  0.00           H
ATOM    583 2HD1 LEU    88      92.580 100.904  96.672  1.00  0.00           H
ATOM    584 3HD1 LEU    88      91.798  99.496  95.915  1.00  0.00           H
ATOM    585 1HD1 LEU    88      90.851 100.605  96.935  1.00  0.00           H
ATOM    586 2HD2 LEU    88      91.004  97.492  97.449  1.00  0.00           H
ATOM    587 3HD2 LEU    88      91.192  97.637  99.211  1.00  0.00           H
ATOM    588 1HD2 LEU    88      90.055  98.690  98.359  1.00  0.00           H
ATOM    589  N   LEU    89      96.626  97.224  99.109  1.00  0.00           N
ATOM    590  CA  LEU    89      97.699  96.192  99.214  1.00  0.00           C
ATOM    591  C   LEU    89      97.562  95.227 100.455  1.00  0.00           C
ATOM    592  O   LEU    89      97.664  94.008 100.298  1.00  0.00           O
ATOM    593  CB  LEU    89      99.055  96.960  99.166  1.00  0.00           C
ATOM    594  CG  LEU    89     100.327  96.091  98.994  1.00  0.00           C
ATOM    595  CD1 LEU    89     100.467  95.560  97.558  1.00  0.00           C
ATOM    596  CD2 LEU    89     101.587  96.896  99.355  1.00  0.00           C
ATOM    597  H   LEU    89      96.766  98.189  99.426  1.00  0.00           H
ATOM    598  HA  LEU    89      97.643  95.547  98.314  1.00  0.00           H
ATOM    599 1HB  LEU    89      99.038  97.716  98.354  1.00  0.00           H
ATOM    600 2HB  LEU    89      99.142  97.561 100.093  1.00  0.00           H
ATOM    601  HG  LEU    89     100.270  95.225  99.684  1.00  0.00           H
ATOM    602 2HD1 LEU    89      99.536  95.099  97.181  1.00  0.00           H
ATOM    603 3HD1 LEU    89     100.723  96.351  96.834  1.00  0.00           H
ATOM    604 1HD1 LEU    89     101.247  94.781  97.489  1.00  0.00           H
ATOM    605 2HD2 LEU    89     101.702  97.797  98.723  1.00  0.00           H
ATOM    606 3HD2 LEU    89     101.562  97.237 100.406  1.00  0.00           H
ATOM    607 1HD2 LEU    89     102.507  96.295  99.239  1.00  0.00           H
ATOM    608  N   LEU    90      97.330  95.750 101.676  1.00  0.00           N
ATOM    609  CA  LEU    90      97.169  94.928 102.915  1.00  0.00           C
ATOM    610  C   LEU    90      95.928  93.965 102.973  1.00  0.00           C
ATOM    611  O   LEU    90      96.098  92.800 103.340  1.00  0.00           O
ATOM    612  CB  LEU    90      97.194  95.890 104.141  1.00  0.00           C
ATOM    613  CG  LEU    90      98.552  96.556 104.496  1.00  0.00           C
ATOM    614  CD1 LEU    90      98.334  97.715 105.480  1.00  0.00           C
ATOM    615  CD2 LEU    90      99.545  95.556 105.115  1.00  0.00           C
ATOM    616  H   LEU    90      97.315  96.778 101.696  1.00  0.00           H
ATOM    617  HA  LEU    90      98.046  94.258 102.994  1.00  0.00           H
ATOM    618 1HB  LEU    90      96.424  96.670 103.982  1.00  0.00           H
ATOM    619 2HB  LEU    90      96.838  95.348 105.041  1.00  0.00           H
ATOM    620  HG  LEU    90      99.004  96.976 103.574  1.00  0.00           H
ATOM    621 2HD1 LEU    90      97.669  98.489 105.053  1.00  0.00           H
ATOM    622 3HD1 LEU    90      97.880  97.378 106.432  1.00  0.00           H
ATOM    623 1HD1 LEU    90      99.284  98.222 105.733  1.00  0.00           H
ATOM    624 2HD2 LEU    90      99.137  95.070 106.021  1.00  0.00           H
ATOM    625 3HD2 LEU    90      99.817  94.752 104.408  1.00  0.00           H
ATOM    626 1HD2 LEU    90     100.488  96.050 105.410  1.00  0.00           H
ATOM    627  N   LYS    91      94.703  94.420 102.640  0.00  0.00           N
ATOM    628  CA  LYS    91      93.473  93.563 102.662  0.00  0.00           C
ATOM    629  C   LYS    91      93.508  92.243 101.787  0.00  0.00           C
ATOM    630  O   LYS    91      93.266  91.185 102.376  0.00  0.00           O
ATOM    631  CB  LYS    91      92.218  94.452 102.398  0.00  0.00           C
ATOM    632  CG  LYS    91      91.542  95.092 103.637  0.00  0.00           C
ATOM    633  CD  LYS    91      92.338  96.229 104.304  0.00  0.00           C
ATOM    634  CE  LYS    91      91.582  96.846 105.488  0.00  0.00           C
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ATOM    635  NZ  LYS    91      92.386  97.929 106.087  0.00  0.00           N
ATOM    636 1HZ  LYS    91      91.873  98.339 106.881  1.00  0.00           H
ATOM    637 2HZ  LYS    91      93.283  97.549 106.419  1.00  0.00           H
ATOM    638 3HZ  LYS    91      92.562  98.657 105.380  1.00  0.00           H
ATOM    639  H   LYS    91      94.687  95.406 102.350  0.00  0.00           H
ATOM    640  HA  LYS    91      93.377  93.183 103.699  0.00  0.00           H
ATOM    641 1HB  LYS    91      91.440  93.828 101.916  0.00  0.00           H
ATOM    642 2HB  LYS    91      92.435  95.229 101.637  0.00  0.00           H
ATOM    643 1HG  LYS    91      91.314  94.304 104.382  0.00  0.00           H
ATOM    644 2HG  LYS    91      90.551  95.483 103.331  0.00  0.00           H
ATOM    645 1HD  LYS    91      92.559  97.007 103.551  0.00  0.00           H
ATOM    646 2HD  LYS    91      93.322  95.847 104.640  0.00  0.00           H
ATOM    647 1HE  LYS    91      91.361  96.077 106.256  0.00  0.00           H
ATOM    648 2HE  LYS    91      90.598  97.243 105.168  0.00  0.00           H
ATOM    649  N   PRO    92      93.817  92.198 100.453  1.00  0.00           N
ATOM    650  CA  PRO    92      94.036  90.912  99.718  1.00  0.00           C
ATOM    651  C   PRO    92      95.423  90.180  99.890  1.00  0.00           C
ATOM    652  O   PRO    92      95.793  89.369  99.038  1.00  0.00           O
ATOM    653  CB  PRO    92      93.768  91.398  98.277  1.00  0.00           C
ATOM    654  CG  PRO    92      94.319  92.824  98.235  1.00  0.00           C
ATOM    655  CD  PRO    92      93.992  93.397  99.612  1.00  0.00           C
ATOM    656  HA  PRO    92      93.260  90.170  99.994  1.00  0.00           H
ATOM    657 1HB  PRO    92      94.220  90.748  97.504  1.00  0.00           H
ATOM    658 2HB  PRO    92      92.679  91.403  98.076  1.00  0.00           H
ATOM    659 1HG  PRO    92      95.417  92.815  98.087  1.00  0.00           H
ATOM    660 2HG  PRO    92      93.897  93.431  97.411  1.00  0.00           H
ATOM    661 1HD  PRO    92      94.812  94.049  99.968  1.00  0.00           H
ATOM    662 2HD  PRO    92      93.067  94.003  99.577  1.00  0.00           H
ATOM    663  N   HIS    93      96.172  90.428 100.981  1.00  0.00           N
ATOM    664  CA  HIS    93      97.474  89.747 101.304  1.00  0.00           C
ATOM    665  C   HIS    93      98.649  89.921 100.264  1.00  0.00           C
ATOM    666  O   HIS    93      99.418  88.994  99.993  1.00  0.00           O
ATOM    667  CB  HIS    93      97.234  88.275 101.763  1.00  0.00           C
ATOM    668  CG  HIS    93      96.378  88.105 103.018  1.00  0.00           C
ATOM    669  ND1 HIS    93      96.872  88.240 104.307  1.00  0.00           N
ATOM    670  CE1 HIS    93      95.697  88.123 105.005  1.00  0.00           C
ATOM    671  NE2 HIS    93      94.519  87.915 104.337  1.00  0.00           N
ATOM    672  CD2 HIS    93      94.985  87.921 103.034  1.00  0.00           C
ATOM    673  H   HIS    93      95.706  91.058 101.647  1.00  0.00           H
ATOM    674  HA  HIS    93      97.865  90.269 102.198  1.00  0.00           H
ATOM    675 1HB  HIS    93      96.801  87.691 100.929  1.00  0.00           H
ATOM    676 2HB  HIS    93      98.208  87.786 101.958  1.00  0.00           H
ATOM    677  HE1 HIS    93      95.706  88.228 106.083  1.00  0.00           H
ATOM    678  HE2 HIS    93      93.557  87.930 104.690  1.00  0.00           H
ATOM    679  HD2 HIS    93      94.367  87.869 102.148  1.00  0.00           H
ATOM    680  N   GLN    94      98.823  91.137  99.720  0.00  0.00           N
ATOM    681  CA  GLN    94      99.797  91.412  98.619  0.00  0.00           C
ATOM    682  C   GLN    94     101.180  92.046  99.017  0.00  0.00           C
ATOM    683  O   GLN    94     102.059  92.109  98.155  0.00  0.00           O
ATOM    684  CB  GLN    94      99.060  92.295  97.574  0.00  0.00           C
ATOM    685  CG  GLN    94      97.975  91.596  96.709  0.00  0.00           C
ATOM    686  CD  GLN    94      97.355  92.477  95.614  0.00  0.00           C
ATOM    687  OE1 GLN    94      97.667  93.647  95.421  0.00  0.00           O
ATOM    688  NE2 GLN    94      96.472  91.924  94.827  0.00  0.00           N
ATOM    689  H   GLN    94      98.058  91.789  99.942  0.00  0.00           H
ATOM    690  HA  GLN    94     100.067  90.467  98.106  0.00  0.00           H
ATOM    691 1HB  GLN    94      99.805  92.722  96.876  0.00  0.00           H
ATOM    692 2HB  GLN    94      98.619  93.181  98.071  0.00  0.00           H
ATOM    693 1HG  GLN    94      97.166  91.217  97.361  0.00  0.00           H
ATOM    694 2HG  GLN    94      98.111  90.700  96.231  0.00  0.00           H
ATOM    695 1HE2 GLN    94      96.379  90.970  94.915  0.00  0.00           H
ATOM    696 2HE2 GLN    94      91.371  90.109  94.015  0.00  0.00           H
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ATOM    708  HE  ARG    95     105.252  95.916 103.996  1.00  0.00           H
ATOM    709  H   ARG    95     100.593  92.395 100.878  1.00  0.00           H
ATOM    710  HA  ARG    95     102.788  94.078 100.097  1.00  0.00           H
ATOM    711 1HB  ARG    95     101.543  94.148 102.272  1.00  0.00           H
ATOM    712 2HB  ARG    95     102.374  92.691 102.810  1.00  0.00           H
ATOM    713 1HG  ARG    95     104.606  93.950 102.667  1.00  0.00           H
ATOM    714 2HG  ARG    95     103.748  95.395 102.145  1.00  0.00           H
ATOM    715 1HD  ARG    95     102.448  95.423 104.319  1.00  0.00           H
ATOM    716 2HD  ARG    95     103.278  93.931 104.835  1.00  0.00           H
ATOM    717 2HH1 ARG    95     103.101  95.282 106.651  1.00  0.00           H
ATOM    718 1HH1 ARG    95     104.170  96.209 107.835  1.00  0.00           H
ATOM    719 1HH2 ARG    95     106.362  96.872 105.340  1.00  0.00           H
ATOM    720 2HH2 ARG    95     105.945  97.078 107.131  1.00  0.00           H
ATOM    721  N   GLU    96     104.096  91.080 100.833  0.00  0.00           N
ATOM    722  CA  GLU    96     105.189  90.147 100.412  0.00  0.00           C
ATOM    723  C   GLU    96     104.931  89.350  99.079  0.00  0.00           C
ATOM    724  O   GLU    96     105.894  88.989  98.402  0.00  0.00           O
ATOM    725  CB  GLU    96     105.463  89.164 101.587  0.00  0.00           C
ATOM    726  CG  GLU    96     106.066  89.793 102.872  0.00  0.00           C
ATOM    727  CD  GLU    96     106.233  88.802 104.017  0.00  0.00           C
ATOM    728  OE1 GLU    96     105.377  88.590 104.869  0.00  0.00           O
ATOM    729  OE2 GLU    96     107.438  88.174 103.990  0.00  0.00           O
ATOM    730  H   GLU    96     103.250  90.754 101.306  0.00  0.00           H
ATOM    731  HA  GLU    96     106.124  90.718 100.229  0.00  0.00           H
ATOM    732 1HB  GLU    96     106.166  88.381 101.235  0.00  0.00           H
ATOM    733 2HB  GLU    96     104.534  88.612 101.832  0.00  0.00           H
ATOM    734 1HG  GLU    96     105.426  90.617 103.237  0.00  0.00           H
ATOM    735 2HG  GLU    96     107.044  90.260 102.651  0.00  0.00           H
ATOM    736  N   LYS    97     103.671  89.057  98.688  0.00  0.00           N
ATOM    737  CA  LYS    97     103.353  88.216  97.488  0.00  0.00           C
ATOM    738  C   LYS    97     103.443  88.919  96.085  0.00  0.00           C
ATOM    739  O   LYS    97     104.022  88.356  95.154  0.00  0.00           O
ATOM    740  CB  LYS    97     101.948  87.561  97.656  0.00  0.00           C
ATOM    741  CG  LYS    97     101.708  86.653  98.883  0.00  0.00           C
ATOM    742  CD  LYS    97     100.329  85.964  98.808  0.00  0.00           C
ATOM    743  CE  LYS    97      99.974  85.222 100.102  0.00  0.00           C
ATOM    744  NZ  LYS    97      98.655  84.577  99.947  0.00  0.00           N
ATOM    745 1HZ  LYS    97      98.413  84.076 100.815  1.00  0.00           H
ATOM    746 2HZ  LYS    97      97.942  85.294  99.755  1.00  0.00           H
ATOM    747 3HZ  LYS    97      98.690  83.908  99.164  1.00  0.00           H
ATOM    748  H   LYS    97     102.948  89.411  99.318  0.00  0.00           H
ATOM    749  HA  LYS    97     104.088  87.389  97.445  0.00  0.00           H
ATOM    750 1HB  LYS    97     101.171  88.351  97.642  0.00  0.00           H
ATOM    751 2HB  LYS    97     101.748  86.960  96.746  0.00  0.00           H
ATOM    752 1HG  LYS    97     102.512  85.895  98.965  0.00  0.00           H
ATOM    753 2HG  LYS    97     101.772  87.260  99.808  0.00  0.00           H
ATOM    754 1HD  LYS    97      99.549  86.725  98.598  0.00  0.00           H
ATOM    755 2HD  LYS    97     100.312  85.270  97.945  0.00  0.00           H
ATOM    756 1HE  LYS    97     100.743  84.464 100.353  0.00  0.00           H
ATOM    757 2HE  LYS    97      99.946  85.926 100.959  0.00  0.00           H
ATOM    758  N   MET    98     102.791  90.083  95.914  0.00  0.00           N
ATOM    759  CA  MET    98     102.786  90.853  94.632  0.00  0.00           C
ATOM    760  C   MET    98     103.722  92.109  94.646  0.00  0.00           C
ATOM    761  O   MET    98     104.487  92.313  93.699  0.00  0.00           O
ATOM    762  CB  MET    98     101.318  91.226  94.282  0.00  0.00           C
ATOM    763  CG  MET    98     100.475  90.087  93.674  0.00  0.00           C
ATOM    764  SD  MET    98      98.916  90.757  93.075  0.00  0.00           S
ATOM    765  CE  MET    98      98.221  89.275  92.335  0.00  0.00           C
ATOM    766  H   MET    98     102.511  90.501  96.807  0.00  0.00           H
ATOM    767  HA  MET    98     103.171  90.224  93.803  0.00  0.00           H
ATOM    768 1HB  MET    98     100.800  91.647  95.163  0.00  0.00           H
ATOM    769 2HB  MET    98     101.318  92.056  93.554  0.00  0.00           H
ATOM    770 1HG  MET    98     101.006  89.617  92.825  0.00  0.00           H
ATOM    771 2HG  MET    98     100.289  89.287  94.414  0.00  0.00           H
ATOM    772 1HE  MET    98      98.818  88.972  91.457  0.00  0.00           H
ATOM    773 2HE  MET    98      97.185  89.464  92.000  0.00  0.00           H
ATOM    774 3HE  MET    98      98.208  88.439  93.057  0.00  0.00           H
ATOM    775  N   SER    99     103.680  92.944  95.705  0.00  0.00           N
ATOM    776  CA  SER    99     104.779  93.904  95.997  0.00  0.00           C
ATOM    777  C   SER    99     106.098  93.204  96.500  0.00  0.00           C
ATOM    778  O   SER    99     106.170  91.989  96.692  0.00  0.00           O
ATOM    779  CB  SER    99     104.199  94.965  96.962  0.00  0.00           C
ATOM    780  OG  SER    99     105.102  96.061  97.138  0.00  0.00           O
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ATOM	781	H	SER	99	103.120	92.555	96.475	0.00	0.00	H
ATOM	782	HA	SER	99	105.037	94.431	95.057	0.00	0.00	H
ATOM	783	1HB	SER	99	103.243	95.360	96.567	0.00	0.00	H
ATOM	784	2HB	SER	99	103.965	94.501	97.940	0.00	0.00	H
ATOM	785	HG	SER	99	104.767	96.590	97.870	0.00	0.00	H
ATOM	786	N	MET	100	107.175	93.992	96.592	1.00	0.00	N
ATOM	787	CA	MET	100	108.594	93.499	96.645	1.00	0.00	C
ATOM	788	C	MET	100	109.244	93.032	95.286	1.00	0.00	C
ATOM	789	O	MET	100	110.469	92.898	95.226	1.00	0.00	O
ATOM	790	CB	MET	100	108.921	92.578	97.861	1.00	0.00	C
ATOM	791	CG	MET	100	108.700	93.223	99.246	1.00	0.00	C
ATOM	792	SD	MET	100	109.201	92.084	100.548	1.00	0.00	S
ATOM	793	CE	MET	100	108.896	93.143	101.971	1.00	0.00	C
ATOM	794	H	MET	100	106.918	94.984	96.637	1.00	0.00	H
ATOM	795	HA	MET	100	109.184	94.413	96.850	1.00	0.00	H
ATOM	796	1HB	MET	100	108.342	91.636	97.792	1.00	0.00	H
ATOM	797	2HB	MET	100	109.979	92.253	97.800	1.00	0.00	H
ATOM	798	1HG	MET	100	109.273	94.163	99.344	1.00	0.00	H
ATOM	799	2HG	MET	100	107.633	93.478	99.390	1.00	0.00	H
ATOM	800	1HE	MET	100	109.507	94.061	101.915	1.00	0.00	H
ATOM	801	3HE	MET	100	107.830	93.435	102.019	1.00	0.00	H
ATOM	802	2HE	MET	100	109.152	92.615	102.907	1.00	0.00	H
ATOM	803	N	GLU	101	108.496	92.944	94.163	0.00	0.00	N
ATOM	804	CA	GLU	101	109.067	92.992	92.774	0.00	0.00	C
ATOM	805	C	GLU	101	110.071	94.151	92.406	0.00	0.00	C
ATOM	806	O	GLU	101	110.931	93.963	91.547	0.00	0.00	O
ATOM	807	CB	GLU	101	107.894	92.894	91.754	0.00	0.00	C
ATOM	808	CG	GLU	101	106.842	94.060	91.838	0.00	0.00	C
ATOM	809	CD	GLU	101	106.279	94.737	90.600	0.00	0.00	C
ATOM	810	OE1	GLU	101	105.843	94.086	89.632	0.00	0.00	O
ATOM	811	OE2	GLU	101	106.170	95.980	90.633	0.00	0.00	O
ATOM	812	H	GLU	101	107.491	92.835	94.351	0.00	0.00	H
ATOM	813	HA	GLU	101	109.663	92.066	92.653	0.00	0.00	H
ATOM	814	1HB	GLU	101	107.339	91.952	91.938	0.00	0.00	H
ATOM	815	2HB	GLU	101	108.294	92.806	90.725	0.00	0.00	H
ATOM	816	1HG	GLU	101	107.241	94.883	92.455	0.00	0.00	H
ATOM	817	2HG	GLU	101	105.963	93.712	92.397	0.00	0.00	H
ATOM	818	N	ILE	102	110.011	95.307	93.091	0.00	0.00	N
ATOM	819	CA	ILE	102	111.117	96.324	93.126	0.00	0.00	C
ATOM	820	C	ILE	102	112.564	95.800	93.464	0.00	0.00	C
ATOM	821	O	ILE	102	113.523	96.238	92.831	0.00	0.00	O
ATOM	822	CB	ILE	102	110.710	97.558	94.018	0.00	0.00	C
ATOM	823	CG2	ILE	102	109.536	98.355	93.396	0.00	0.00	C
ATOM	824	CG1	ILE	102	110.409	97.228	95.514	0.00	0.00	C
ATOM	825	CD1	ILE	102	110.410	98.432	96.472	0.00	0.00	C
ATOM	826	H	ILE	102	109.270	95.297	93.797	0.00	0.00	H
ATOM	827	HA	ILE	102	111.220	96.704	92.090	0.00	0.00	H
ATOM	828	HB	ILE	102	111.585	98.242	94.004	0.00	0.00	H
ATOM	829	1HG2	ILE	102	109.385	99.330	93.894	0.00	0.00	H
ATOM	830	2HG2	ILE	102	109.710	98.570	92.327	0.00	0.00	H
ATOM	831	3HG2	ILE	102	108.578	97.804	93.456	0.00	0.00	H
ATOM	832	1HG1	ILE	102	111.165	96.515	95.895	0.00	0.00	H
ATOM	833	2HG1	ILE	102	109.448	96.687	95.601	0.00	0.00	H
ATOM	834	1HD1	ILE	102	110.241	98.116	97.517	0.00	0.00	H
ATOM	835	2HD1	ILE	102	111.381	98.963	96.454	0.00	0.00	H
ATOM	836	3HD1	ILE	102	109.623	99.168	96.227	0.00	0.00	H
ATOM	837	N	SER	103	112.731	94.840	94.395	1.00	0.00	N
ATOM	838	CA	SER	103	114.010	94.078	94.548	1.00	0.00	C
ATOM	839	C	SER	103	114.107	93.001	93.393	1.00	0.00	C
ATOM	840	O	SER	103	115.580	92.714	93.302	1.00	0.00	O
ATOM	841	CB	SER	103	113.946	93.347	95.903	1.00	0.00	C
ATOM	842	OG	SER	103	115.212	93.703	95.333	1.00	0.00	O

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ATOM    854  CG1 ILE   104     112.175  89.917  92.006  0.00  0.00           C
ATOM    855  CD1 ILE   104     110.818  89.209  91.806  0.00  0.00           C
ATOM    856  H   ILE   104     112.552  93.098  92.676  0.00  0.00           H
ATOM    857  HA  ILE   104     114.641  91.231  91.467  0.00  0.00           H
ATOM    858  HB  ILE   104     111.688  91.577  90.702  0.00  0.00           H
ATOM    859 1HG2 ILE   104     112.044  89.477  89.301  0.00  0.00           H
ATOM    860 2HG2 ILE   104     112.997  90.835  88.724  0.00  0.00           H
ATOM    861 3HG2 ILE   104     113.784  89.541  89.662  0.00  0.00           H
ATOM    862 1HG1 ILE   104     112.122  90.432  92.984  0.00  0.00           H
ATOM    863 2HG1 ILE   104     112.976  89.162  92.138  0.00  0.00           H
ATOM    864 1HD1 ILE   104     110.546  88.603  92.691  0.00  0.00           H
ATOM    865 2HD1 ILE   104     109.990  89.923  91.641  0.00  0.00           H
ATOM    866 3HD1 ILE   104     110.825  88.518  90.944  0.00  0.00           H
ATOM    867  N   HIS   105     113.344  93.746  89.616  1.00  0.00           N
ATOM    868  CA  HIS   105     113.695  94.702  88.517  1.00  0.00           C
ATOM    869  C   HIS   105     114.587  95.965  88.831  1.00  0.00           C
ATOM    870  O   HIS   105     114.998  96.646  87.890  1.00  0.00           O
ATOM    871  CB  HIS   105     112.403  95.005  87.708  1.00  0.00           C
ATOM    872  CG  HIS   105     111.208  95.654  88.402  1.00  0.00           C
ATOM    873  ND1 HIS   105     109.950  95.079  88.433  1.00  0.00           N
ATOM    874  CE1 HIS   105     109.254  96.094  89.029  1.00  0.00           C
ATOM    875  NE2 HIS   105     109.900  97.248  89.378  1.00  0.00           N
ATOM    876  CD2 HIS   105     111.175  96.940  88.946  1.00  0.00           C
ATOM    877  H   HIS   105     112.395  93.691  90.011  1.00  0.00           H
ATOM    878  HA  HIS   105     114.335  94.144  87.803  1.00  0.00           H
ATOM    879 1HB  HIS   105     112.660  95.634  86.835  1.00  0.00           H
ATOM    880 2HB  HIS   105     112.066  94.058  87.248  1.00  0.00           H
ATOM    881  HE1 HIS   105     108.185  95.999  89.157  1.00  0.00           H
ATOM    882  HE2 HIS   105     109.511  98.124  89.737  1.00  0.00           H
ATOM    883  HD2 HIS   105     112.024  97.602  88.960  1.00  0.00           H
ATOM    884  N   ARG   106     114.967  96.248  90.091  1.00  0.00           N
ATOM    885  CA  ARG   106     116.188  97.062  90.403  1.00  0.00           C
ATOM    886  C   ARG   106     117.561  96.302  90.234  1.00  0.00           C
ATOM    887  O   ARG   106     118.534  96.905  89.777  1.00  0.00           O
ATOM    888  CB  ARG   106     116.016  97.669  91.825  1.00  0.00           C
ATOM    889  CG  ARG   106     116.944  98.849  92.215  1.00  0.00           C
ATOM    890  CD  ARG   106     116.548 100.176  91.548  1.00  0.00           C
ATOM    891  NE  ARG   106     117.304 101.306  92.139  1.00  0.00           N
ATOM    892  CZ  ARG   106     117.196 102.573  91.754  1.00  0.00           C
ATOM    893  NH1 ARG   106     116.436 102.985  90.782  1.00  0.00           N
ATOM    894  NH2 ARG   106     117.895 103.444  92.389  1.00  0.00           N
ATOM    895  HE  ARG   106     117.960 101.093  92.904  1.00  0.00           H
ATOM    896  H   ARG   106     114.499  95.669  90.799  1.00  0.00           H
ATOM    897  HA  ARG   106     116.232  97.909  89.690  1.00  0.00           H
ATOM    898 1HB  ARG   106     114.973  98.014  91.962  1.00  0.00           H
ATOM    899 2HB  ARG   106     116.131  96.860  92.572  1.00  0.00           H
ATOM    900 1HG  ARG   106     116.907  98.977  93.315  1.00  0.00           H
ATOM    901 2HG  ARG   106     118.005  98.616  91.995  1.00  0.00           H
ATOM    902 1HD  ARG   106     116.720 100.122  90.454  1.00  0.00           H
ATOM    903 2HD  ARG   106     115.467 100.362  91.693  1.00  0.00           H
ATOM    904 2HH1 ARG   106     115.966 102.231  90.280  1.00  0.00           H
ATOM    905 1HH1 ARG   106     116.449 103.981  90.557  1.00  0.00           H
ATOM    906 1HH2 ARG   106     118.476 103.015  93.111  1.00  0.00           H
ATOM    907 2HH2 ARG   106     117.837 104.410  92.071  1.00  0.00           H
ATOM    908  N   SER   107     117.656  95.006  90.591  1.00  0.00           N
ATOM    909  CA  SER   107     118.898  94.191  90.412  1.00  0.00           C
ATOM    910  C   SER   107     119.231  93.611  88.983  1.00  0.00           C
ATOM    911  O   SER   107     120.313  93.038  88.811  1.00  0.00           O
ATOM    912  CB  SER   107     118.801  93.051  91.457  1.00  0.00           C
ATOM    913  OG  SER   107     120.020  92.306  91.515  1.00  0.00           O
ATOM    914  H   SER   107     116.758  94.573  90.835  1.00  0.00           H
ATOM    915  HA  SER   107     119.773  94.811  90.692  1.00  0.00           H
ATOM    916 1HB  SER   107     118.583  93.450  92.468  1.00  0.00           H
ATOM    917 2HB  SER   107     117.956  92.371  91.219  1.00  0.00           H
ATOM    918  HG  SER   107     120.314  92.177  90.601  1.00  0.00           H
ATOM    919  N   LEU   108     118.339  93.708  87.985  1.00  0.00           N
ATOM    920  CA  LEU   108     118.502  93.046  86.658  1.00  0.00           C
ATOM    921  C   LEU   108     119.119  94.006  85.584  1.00  0.00           C
ATOM    922  O   LEU   108     118.409  94.660  84.814  1.00  0.00           O
ATOM    923  CB  LEU   108     117.098  92.487  86.259  1.00  0.00           C
ATOM    924  CG  LEU   108     116.686  91.054  86.710  1.00  0.00           C
ATOM    925  CD1 LEU   108     117.204  90.574  88.077  1.00  0.00           C
ATOM    926  CD2 LEU   108     115.152  90.965  86.708  1.00  0.00           C
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ATOM	927	H	LEU	108	117.463	94.155	88.273	1.00	0.00	H
ATOM	928	HA	LEU	108	119.184	92.174	86.733	1.00	0.00	H
ATOM	929	1HB	LEU	108	116.324	93.229	86.542	1.00	0.00	H
ATOM	930	2HB	LEU	108	117.022	92.480	85.156	1.00	0.00	H
ATOM	931	HG	LEU	108	117.076	90.334	85.960	1.00	0.00	H
ATOM	932	2HD1	LEU	108	119.307	90.517	88.100	1.00	0.00	H
ATOM	933	3HD1	LEU	108	116.898	91.239	88.903	1.00	0.00	H
ATOM	934	1HD1	LEU	108	116.842	89.558	88.321	1.00	0.00	H
ATOM	935	2HD2	LEU	108	114.700	91.680	87.419	1.00	0.00	H
ATOM	936	3HD2	LEU	108	114.728	91.191	85.712	1.00	0.00	H
ATOM	937	1HD2	LEU	108	114.791	89.961	86.993	1.00	0.00	H
ATOM	938	N	ALA	109	120.459	94.046	85.502	1.00	0.00	N
ATOM	939	CA	ALA	109	121.181	94.809	84.450	1.00	0.00	C
ATOM	940	C	ALA	109	121.276	94.026	83.092	1.00	0.00	C
ATOM	941	O	ALA	109	122.205	93.242	82.864	1.00	0.00	O
ATOM	942	CB	ALA	109	122.549	95.166	85.065	1.00	0.00	C
ATOM	943	H	ALA	109	120.937	93.517	86.238	1.00	0.00	H
ATOM	944	HA	ALA	109	120.661	95.770	84.261	1.00	0.00	H
ATOM	945	2HB	ALA	109	122.442	95.760	85.993	1.00	0.00	H
ATOM	946	3HB	ALA	109	123.147	94.269	85.313	1.00	0.00	H
ATOM	947	1HB	ALA	109	123.155	95.773	84.367	1.00	0.00	H
ATOM	948	N	HIS	110	120.281	94.224	82.211	0.00	0.00	N
ATOM	949	CA	HIS	110	120.183	93.522	80.899	0.00	0.00	C
ATOM	950	C	HIS	110	119.536	94.431	79.796	0.00	0.00	C
ATOM	951	O	HIS	110	118.774	95.359	80.081	0.00	0.00	O
ATOM	952	CB	HIS	110	119.385	92.201	81.129	0.00	0.00	C
ATOM	953	CG	HIS	110	119.470	91.154	80.018	0.00	0.00	C
ATOM	954	ND1	HIS	110	118.360	90.593	79.403	0.00	0.00	N
ATOM	955	CE1	HIS	110	118.990	89.661	78.619	0.00	0.00	C
ATOM	956	NE2	HIS	110	120.356	89.578	78.616	0.00	0.00	N
ATOM	957	CD2	HIS	110	120.651	90.545	79.559	0.00	0.00	C
ATOM	958	H	HIS	110	119.499	94.777	82.586	0.00	0.00	H
ATOM	959	HA	HIS	110	121.208	93.272	80.555	0.00	0.00	H
ATOM	960	1HB	HIS	110	118.324	92.438	81.344	0.00	0.00	H
ATOM	961	2HB	HIS	110	119.738	91.705	82.050	0.00	0.00	H
ATOM	962	HE1	HIS	110	118.402	88.948	78.058	0.00	0.00	H
ATOM	963	HE2	HIS	110	120.958	88.868	78.185	0.00	0.00	H
ATOM	964	HD2	HIS	110	121.637	90.755	79.950	0.00	0.00	H
ATOM	965	N	GLN	111	119.796	94.124	78.511	1.00	0.00	N
ATOM	966	CA	GLN	111	119.073	94.767	77.370	1.00	0.00	C
ATOM	967	C	GLN	111	117.522	94.518	77.294	1.00	0.00	C
ATOM	968	O	GLN	111	116.783	95.452	76.977	1.00	0.00	O
ATOM	969	CB	GLN	111	119.814	94.355	76.065	1.00	0.00	C
ATOM	970	CG	GLN	111	119.352	95.115	74.789	1.00	0.00	C
ATOM	971	CD	GLN	111	120.079	94.724	73.503	1.00	0.00	C
ATOM	972	OE1	GLN	111	119.676	93.832	72.768	1.00	0.00	O
ATOM	973	NE2	GLN	111	121.156	95.386	73.167	1.00	0.00	N
ATOM	974	H	GLN	111	120.352	93.273	78.391	1.00	0.00	H
ATOM	975	HA	GLN	111	119.191	95.864	77.481	1.00	0.00	H
ATOM	976	1HB	GLN	111	120.904	94.513	76.190	1.00	0.00	H
ATOM	977	2HB	GLN	111	119.695	93.264	75.901	1.00	0.00	H
ATOM	978	1HG	GLN	111	118.276	94.920	74.613	1.00	0.00	H
ATOM	979	2HG	GLN	111	119.413	96.208	74.943	1.00	0.00	H
ATOM	980	1HE2	GLN	111	121.424	96.166	73.769	1.00	0.00	H
ATOM	981	2HE2	GLN	111	121.540	95.113	72.259	1.00	0.00	H
ATOM	982	N	HIS	112	117.029	93.294	77.559	1.00	0.00	N
ATOM	983	CA	HIS	112	115.593	92.928	77.334	1.00	0.00	C
ATOM	984	C	HIS	112	114.665	93.099	78.602	1.00	0.00	C
ATOM	985	O	HIS	112	113.745	92.309	78.828	1.00	0.00	O
ATOM	986	CB	HIS	112	115.545	91.483	76.735	1.00	0.00	C
ATOM	987	CG	HIS	112	116.435	91.110	75.527	1.00	0.00	C
ATOM	988	ND1	HIS	112	117.759	93.031	77.502	1.00	0.00	N

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ATOM   1000  CA  VAL   113     114.177  94.363  80.732  1.00  0.00           C
ATOM   1001  C   VAL   113     113.876  95.899  80.839  1.00  0.00           C
ATOM   1002  O   VAL   113     114.762  96.727  80.603  1.00  0.00           O
ATOM   1003  CB  VAL   113     115.031  93.822  81.942  1.00  0.00           C
ATOM   1004  CG1 VAL   113     114.422  94.136  83.330  1.00  0.00           C
ATOM   1005  CG2 VAL   113     115.264  92.290  81.916  1.00  0.00           C
ATOM   1006  H   VAL   113     115.671  94.731  79.141  1.00  0.00           H
ATOM   1007  HA  VAL   113     113.208  93.826  80.741  1.00  0.00           H
ATOM   1008  HB  VAL   113     116.025  94.314  81.899  1.00  0.00           H
ATOM   1009 1HG1 VAL   113     113.405  93.722  83.446  1.00  0.00           H
ATOM   1010 2HG1 VAL   113     115.039  93.742  84.161  1.00  0.00           H
ATOM   1011 3HG1 VAL   113     114.345  95.227  83.509  1.00  0.00           H
ATOM   1012 2HG2 VAL   113     115.809  91.975  81.008  1.00  0.00           H
ATOM   1013 3HG2 VAL   113     115.874  91.945  82.773  1.00  0.00           H
ATOM   1014 1HG2 VAL   113     114.314  91.724  81.936  1.00  0.00           H
ATOM   1015  N   VAL   114     112.642  96.296  81.208  0.00  0.00           N
ATOM   1016  CA  VAL   114     112.230  97.744  81.262  0.00  0.00           C
ATOM   1017  C   VAL   114     113.120  98.550  82.289  0.00  0.00           C
ATOM   1018  O   VAL   114     113.304  98.124  83.436  0.00  0.00           O
ATOM   1019  CB  VAL   114     110.701  97.852  81.615  0.00  0.00           C
ATOM   1020  CG1 VAL   114     110.200  99.308  81.734  0.00  0.00           C
ATOM   1021  CG2 VAL   114     109.717  97.185  80.624  0.00  0.00           C
ATOM   1022  H   VAL   114     112.016  95.535  81.503  0.00  0.00           H
ATOM   1023  HA  VAL   114     112.370  98.187  80.256  0.00  0.00           H
ATOM   1024  HB  VAL   114     110.557  97.367  82.602  0.00  0.00           H
ATOM   1025 1HG1 VAL   114     110.767  99.897  82.479  0.00  0.00           H
ATOM   1026 2HG1 VAL   114     110.258  99.866  80.780  0.00  0.00           H
ATOM   1027 3HG1 VAL   114     109.150  99.339  82.069  0.00  0.00           H
ATOM   1028 1HG2 VAL   114     109.688  97.697  79.644  0.00  0.00           H
ATOM   1029 2HG2 VAL   114     109.962  96.125  80.438  0.00  0.00           H
ATOM   1030 3HG2 VAL   114     108.678  97.192  81.006  0.00  0.00           H
ATOM   1031  N   GLY   115     113.677  99.701  81.873  1.00  0.00           N
ATOM   1032  CA  GLY   115     114.555 100.527  82.744  1.00  0.00           C
ATOM   1033  C   GLY   115     113.860 101.190  83.956  1.00  0.00           C
ATOM   1034  O   GLY   115     112.941 101.999  83.811  1.00  0.00           O
ATOM   1035  H   GLY   115     113.367 100.067  80.961  1.00  0.00           H
ATOM   1036 1HA  GLY   115     115.441  99.941  83.061  1.00  0.00           H
ATOM   1037 2HA  GLY   115     114.975 101.342  82.130  1.00  0.00           H
ATOM   1038  N   PHE   116     114.284 100.805  85.163  1.00  0.00           N
ATOM   1039  CA  PHE   116     113.653 101.270  86.423  1.00  0.00           C
ATOM   1040  C   PHE   116     114.361 102.526  87.030  1.00  0.00           C
ATOM   1041  O   PHE   116     115.506 102.470  87.485  1.00  0.00           O
ATOM   1042  CB  PHE   116     113.598 100.040  87.373  1.00  0.00           C
ATOM   1043  CG  PHE   116     112.797 100.237  88.671  1.00  0.00           C
ATOM   1044  CD1 PHE   116     111.508 100.777  88.644  1.00  0.00           C
ATOM   1045  CE1 PHE   116     110.797 100.954  89.820  1.00  0.00           C
ATOM   1046  CZ  PHE   116     111.341 100.551  91.030  1.00  0.00           C
ATOM   1047  CE2 PHE   116     112.610  99.980  91.072  1.00  0.00           C
ATOM   1048  CD2 PHE   116     113.338  99.830  89.893  1.00  0.00           C
ATOM   1049  H   PHE   116     114.915  99.996  85.144  1.00  0.00           H
ATOM   1050  HA  PHE   116     112.602 101.542  86.204  1.00  0.00           H
ATOM   1051 1HB  PHE   116     113.152  99.173  86.844  1.00  0.00           H
ATOM   1052 2HB  PHE   116     114.633  99.711  87.601  1.00  0.00           H
ATOM   1053  HD1 PHE   116     111.048 101.070  87.714  1.00  0.00           H
ATOM   1054  HE1 PHE   116     109.818 101.392  89.786  1.00  0.00           H
ATOM   1055  HZ  PHE   116     110.760 100.687  91.925  1.00  0.00           H
ATOM   1056  HE2 PHE   116     113.026  99.647  92.013  1.00  0.00           H
ATOM   1057  HD2 PHE   116     114.313  99.368  89.922  1.00  0.00           H
ATOM   1058  N   HIS   117     113.642 103.657  87.050  1.00  0.00           N
ATOM   1059  CA  HIS   117     114.145 104.947  87.595  1.00  0.00           C
ATOM   1060  C   HIS   117     114.102 105.098  89.160  1.00  0.00           C
ATOM   1061  O   HIS   117     115.055 105.637  89.731  1.00  0.00           O
ATOM   1062  CB  HIS   117     113.346 106.045  86.836  1.00  0.00           C
ATOM   1063  CG  HIS   117     113.832 107.481  87.004  1.00  0.00           C
ATOM   1064  ND1 HIS   117     113.032 108.504  87.493  1.00  0.00           N
ATOM   1065  CE1 HIS   117     113.899 109.556  87.340  1.00  0.00           C
ATOM   1066  NE2 HIS   117     115.144 109.346  86.812  1.00  0.00           N
ATOM   1067  CD2 HIS   117     115.081 107.982  86.595  1.00  0.00           C
ATOM   1068  H   HIS   117     112.668 103.548  86.734  1.00  0.00           H
ATOM   1069  HA  HIS   117     115.213 105.053  87.312  1.00  0.00           H
ATOM   1070 1HB  HIS   117     113.342 105.837  85.749  1.00  0.00           H
ATOM   1071 2HB  HIS   117     112.280 105.988  87.128  1.00  0.00           H
ATOM   1072  HE1 HIS   117     113.600 110.546  87.656  1.00  0.00           H
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ATOM	1073	HE2	HIS	117	115.907	110.015	86.667	1.00	0.00	H
ATOM	1074	HD2	HIS	117	115.869	107.380	86.162	1.00	0.00	H
ATOM	1075	N	GLY	118	113.030	104.664	89.853	1.00	0.00	N
ATOM	1076	CA	GLY	118	112.920	104.847	91.324	1.00	0.00	C
ATOM	1077	C	GLY	118	111.772	104.081	92.021	1.00	0.00	C
ATOM	1078	O	GLY	118	110.634	104.043	91.544	1.00	0.00	O
ATOM	1079	H	GLY	118	112.330	104.175	89.282	1.00	0.00	H
ATOM	1080	1HA	GLY	118	113.891	104.600	91.798	1.00	0.00	H
ATOM	1081	2HA	GLY	118	112.763	105.919	91.540	1.00	0.00	H
ATOM	1082	N	PHE	119	112.086	103.527	93.199	1.00	0.00	N
ATOM	1083	CA	PHE	119	111.077	103.036	94.179	1.00	0.00	C
ATOM	1084	C	PHE	119	110.838	104.101	95.301	1.00	0.00	C
ATOM	1085	O	PHE	119	111.701	104.312	96.160	1.00	0.00	O
ATOM	1086	CB	PHE	119	111.485	101.633	94.732	1.00	0.00	C
ATOM	1087	CG	PHE	119	112.841	101.449	95.447	1.00	0.00	C
ATOM	1088	CD1	PHE	119	112.914	101.471	96.843	1.00	0.00	C
ATOM	1089	CE1	PHE	119	114.134	101.278	97.487	1.00	0.00	C
ATOM	1090	CZ	PHE	119	115.288	101.058	96.739	1.00	0.00	C
ATOM	1091	CE2	PHE	119	115.225	101.031	95.348	1.00	0.00	C
ATOM	1092	CD2	PHE	119	114.005	101.220	94.704	1.00	0.00	C
ATOM	1093	H	PHE	119	113.071	103.618	93.465	1.00	0.00	H
ATOM	1094	HA	PHE	119	110.110	102.870	93.664	1.00	0.00	H
ATOM	1095	1HB	PHE	119	110.676	101.288	95.402	1.00	0.00	H
ATOM	1096	2HB	PHE	119	111.447	100.900	93.913	1.00	0.00	H
ATOM	1097	HD1	PHE	119	112.028	101.651	97.436	1.00	0.00	H
ATOM	1098	HE1	PHE	119	114.185	101.302	98.566	1.00	0.00	H
ATOM	1099	HZ	PHE	119	116.236	100.912	97.237	1.00	0.00	H
ATOM	1100	HE2	PHE	119	116.122	100.869	94.767	1.00	0.00	H
ATOM	1101	HD2	PHE	119	113.975	101.198	93.624	1.00	0.00	H
ATOM	1102	N	PHE	120	109.682	104.788	95.304	1.00	0.00	N
ATOM	1103	CA	PHE	120	109.403	105.868	96.300	1.00	0.00	C
ATOM	1104	C	PHE	120	108.310	105.392	97.306	1.00	0.00	C
ATOM	1105	O	PHE	120	107.118	105.356	96.981	1.00	0.00	O
ATOM	1106	CB	PHE	120	109.042	107.233	95.639	1.00	0.00	C
ATOM	1107	CG	PHE	120	109.881	107.724	94.442	1.00	0.00	C
ATOM	1108	CD1	PHE	120	109.235	108.097	93.260	1.00	0.00	C
ATOM	1109	CE1	PHE	120	109.976	108.511	92.159	1.00	0.00	C
ATOM	1110	CZ	PHE	120	111.364	108.551	92.223	1.00	0.00	C
ATOM	1111	CE2	PHE	120	112.017	108.195	93.399	1.00	0.00	C
ATOM	1112	CD2	PHE	120	111.279	107.789	94.510	1.00	0.00	C
ATOM	1113	H	PHE	120	109.077	104.606	94.491	1.00	0.00	H
ATOM	1114	HA	PHE	120	110.320	106.093	96.884	1.00	0.00	H
ATOM	1115	1HB	PHE	120	107.971	107.235	95.375	1.00	0.00	H
ATOM	1116	2HB	PHE	120	109.108	108.011	96.421	1.00	0.00	H
ATOM	1117	HD1	PHE	120	108.157	108.067	93.183	1.00	0.00	H
ATOM	1118	HE1	PHE	120	109.473	108.812	91.255	1.00	0.00	H
ATOM	1119	HZ	PHE	120	111.928	108.856	91.355	1.00	0.00	H
ATOM	1120	HE2	PHE	120	113.096	108.229	93.448	1.00	0.00	H
ATOM	1121	HD2	PHE	120	111.798	107.499	95.411	1.00	0.00	H
ATOM	1122	N	GLU	121	108.716	105.034	98.534	1.00	0.00	N
ATOM	1123	CA	GLU	121	107.772	104.624	99.617	1.00	0.00	C
ATOM	1124	C	GLU	121	107.252	105.878	100.408	1.00	0.00	C
ATOM	1125	O	GLU	121	107.704	106.199	101.511	1.00	0.00	O
ATOM	1126	CB	GLU	121	108.493	103.563	100.497	1.00	0.00	C
ATOM	1127	CG	GLU	121	108.826	102.219	99.790	1.00	0.00	C
ATOM	1128	CD	GLU	121	109.594	101.222	100.647	1.00	0.00	C
ATOM	1129	OE1	GLU	121	110.803	101.042	100.568	1.00	0.00	O
ATOM	1130	OE2	GLU	121	108.785	100.544	101.503	1.00	0.00	O
ATOM	1131	H	GLU	121	109.733	105.042	98.666	1.00	0.00	H
ATOM	1132	HA	GLU	121	106.880	104.122	99.186	1.00	0.00	H
ATOM	1133	1HB	GLU	121	109.416	104.005	100.925	1.00	0.00	H
ATOM	1134	2HB	GLU	121	107.887	103.013	101.370	1.00	0.00	H

ATOM	1146	HA	ASP	122	106.761	108.465	100.784	1.00	0.00	H
ATOM	1147	1HB	ASP	122	104.884	108.341	98.348	1.00	0.00	H
ATOM	1148	2HB	ASP	122	105.175	109.796	99.277	1.00	0.00	H
ATOM	1149	N	ASN	123	104.925	107.982	102.515	1.00	0.00	N
ATOM	1150	CA	ASN	123	103.886	107.675	103.557	1.00	0.00	C
ATOM	1151	C	ASN	123	103.339	106.194	103.514	1.00	0.00	C
ATOM	1152	O	ASN	123	102.127	105.962	103.542	1.00	0.00	O
ATOM	1153	CB	ASN	123	102.752	108.748	103.604	1.00	0.00	C
ATOM	1154	CG	ASN	123	103.189	110.195	103.819	1.00	0.00	C
ATOM	1155	OD1	ASN	123	103.643	110.586	104.886	1.00	0.00	O
ATOM	1156	ND2	ASN	123	103.070	111.034	102.823	1.00	0.00	N
ATOM	1157	H	ASN	123	105.924	108.049	102.740	1.00	0.00	H
ATOM	1158	HA	ASN	123	104.400	107.744	104.536	1.00	0.00	H
ATOM	1159	1HB	ASN	123	102.123	108.658	102.700	1.00	0.00	H
ATOM	1160	2HB	ASN	123	102.063	108.508	104.435	1.00	0.00	H
ATOM	1161	1HD2	ASN	123	103.425	111.971	103.025	1.00	0.00	H
ATOM	1162	2HD2	ASN	123	102.787	110.631	101.927	1.00	0.00	H
ATOM	1163	N	ASP	124	104.237	105.188	103.438	1.00	0.00	N
ATOM	1164	CA	ASP	124	103.882	103.736	103.266	1.00	0.00	C
ATOM	1165	C	ASP	124	103.351	103.261	101.859	1.00	0.00	C
ATOM	1166	O	ASP	124	103.606	102.112	101.488	1.00	0.00	O
ATOM	1167	CB	ASP	124	103.058	103.142	104.444	1.00	0.00	C
ATOM	1168	CG	ASP	124	103.715	103.228	105.818	1.00	0.00	C
ATOM	1169	OD1	ASP	124	104.749	102.645	106.119	1.00	0.00	O
ATOM	1170	OD2	ASP	124	103.021	104.022	106.677	1.00	0.00	O
ATOM	1171	H	ASP	124	105.196	105.526	103.305	1.00	0.00	H
ATOM	1172	HA	ASP	124	104.861	103.217	103.318	1.00	0.00	H
ATOM	1173	1HB	ASP	124	102.065	103.615	104.486	1.00	0.00	H
ATOM	1174	2HB	ASP	124	102.859	102.072	104.258	1.00	0.00	H
ATOM	1175	N	PHE	125	102.625	104.082	101.077	1.00	0.00	N
ATOM	1176	CA	PHE	125	102.218	103.745	99.679	1.00	0.00	C
ATOM	1177	C	PHE	125	103.367	103.892	98.614	1.00	0.00	C
ATOM	1178	O	PHE	125	104.244	104.757	98.716	1.00	0.00	O
ATOM	1179	CB	PHE	125	100.901	104.492	99.325	1.00	0.00	C
ATOM	1180	CG	PHE	125	100.837	106.028	99.414	1.00	0.00	C
ATOM	1181	CD1	PHE	125	100.333	106.635	100.570	1.00	0.00	C
ATOM	1182	CE1	PHE	125	100.190	108.019	100.631	1.00	0.00	C
ATOM	1183	CZ	PHE	125	100.550	108.805	99.539	1.00	0.00	C
ATOM	1184	CE2	PHE	125	101.055	108.208	98.386	1.00	0.00	C
ATOM	1185	CD2	PHE	125	101.200	106.824	98.323	1.00	0.00	C
ATOM	1186	H	PHE	125	102.548	105.039	101.444	1.00	0.00	H
ATOM	1187	HA	PHE	125	101.938	102.672	99.674	1.00	0.00	H
ATOM	1188	1HB	PHE	125	100.599	104.191	98.304	1.00	0.00	H
ATOM	1189	2HB	PHE	125	100.100	104.073	99.960	1.00	0.00	H
ATOM	1190	HD1	PHE	125	100.052	106.040	101.426	1.00	0.00	H
ATOM	1191	HE1	PHE	125	99.803	108.482	101.528	1.00	0.00	H
ATOM	1192	HZ	PHE	125	100.441	109.878	99.588	1.00	0.00	H
ATOM	1193	HE2	PHE	125	101.326	108.821	97.541	1.00	0.00	H
ATOM	1194	HD2	PHE	125	101.594	106.371	97.423	1.00	0.00	H
ATOM	1195	N	VAL	126	103.404	102.985	97.623	1.00	0.00	N
ATOM	1196	CA	VAL	126	104.648	102.689	96.843	1.00	0.00	C
ATOM	1197	C	VAL	126	104.499	103.180	95.362	1.00	0.00	C
ATOM	1198	O	VAL	126	103.635	102.708	94.614	1.00	0.00	O
ATOM	1199	CB	VAL	126	105.031	101.163	96.936	1.00	0.00	C
ATOM	1200	CG1	VAL	126	106.404	100.850	96.290	1.00	0.00	C
ATOM	1201	CG2	VAL	126	105.081	100.582	98.371	1.00	0.00	C
ATOM	1202	H	VAL	126	102.554	102.412	97.532	1.00	0.00	H
ATOM	1203	HA	VAL	126	105.504	103.229	97.296	1.00	0.00	H
ATOM	1204	HB	VAL	126	104.264	100.587	96.380	1.00	0.00	H
ATOM	1205	1HG1	VAL	126	107.235	101.379	96.795	1.00	0.00	H
ATOM	1206	2HG1	VAL	126	106.641	99.769	96.314	1.00	0.00	H
ATOM	1207	3HG1	VAL	126	106.439	101.147	95.225	1.00	0.00	H
ATOM	1208	2HG2	VAL	126	104.092	100.624	98.866	1.00	0.00	H
ATOM	1209	3HG2	VAL	126	105.391	99.521	98.392	1.00	0.00	H
ATOM	1210	1HG2	VAL	126	105.773	101.142	99.025	1.00	0.00	H
ATOM	1211	N	PHE	127	105.383	104.087	94.921	1.00	0.00	N
ATOM	1212	CA	PHE	127	105.474	104.515	93.496	1.00	0.00	C
ATOM	1213	C	PHE	127	106.590	103.719	92.746	1.00	0.00	C
ATOM	1214	O	PHE	127	107.765	103.756	93.129	1.00	0.00	O
ATOM	1215	CB	PHE	127	105.762	106.036	93.415	1.00	0.00	C
ATOM	1216	CG	PHE	127	104.615	106.959	93.846	1.00	0.00	C
ATOM	1217	CD1	PHE	127	104.543	107.434	95.159	1.00	0.00	C
ATOM	1218	CE1	PHE	127	103.508	108.284	95.539	1.00	0.00	C

ATOM	1219	CZ	PHE	127	102.537	108.658	94.615	1.00	0.00	C
ATOM	1220	CE2	PHE	127	102.603	108.186	93.306	1.00	0.00	C
ATOM	1221	CD2	PHE	127	103.636	107.337	92.922	1.00	0.00	C
ATOM	1222	H	PHE	127	105.994	104.480	95.651	1.00	0.00	H
ATOM	1223	HA	PHE	127	104.504	104.346	92.983	1.00	0.00	H
ATOM	1224	1HB	PHE	127	106.677	106.262	93.988	1.00	0.00	H
ATOM	1225	2HB	PHE	127	106.045	106.300	92.376	1.00	0.00	H
ATOM	1226	HD1	PHE	127	105.287	107.144	95.888	1.00	0.00	H
ATOM	1227	HE1	PHE	127	103.464	108.655	96.551	1.00	0.00	H
ATOM	1228	HZ	PHE	127	101.733	109.317	94.911	1.00	0.00	H
ATOM	1229	HE2	PHE	127	101.855	108.475	92.583	1.00	0.00	H
ATOM	1230	HD2	PHE	127	103.676	106.974	91.905	1.00	0.00	H
ATOM	1231	N	VAL	128	106.219	103.025	91.663	1.00	0.00	N
ATOM	1232	CA	VAL	128	107.158	102.171	90.872	1.00	0.00	C
ATOM	1233	C	VAL	128	107.331	102.863	89.474	1.00	0.00	C
ATOM	1234	O	VAL	128	106.446	102.756	88.615	1.00	0.00	O
ATOM	1235	CB	VAL	128	106.594	100.701	90.814	1.00	0.00	C
ATOM	1236	CG1	VAL	128	107.465	99.721	89.999	1.00	0.00	C
ATOM	1237	CG2	VAL	128	106.366	100.039	92.194	1.00	0.00	C
ATOM	1238	H	VAL	128	105.201	103.006	91.501	1.00	0.00	H
ATOM	1239	HA	VAL	128	108.153	102.117	91.363	1.00	0.00	H
ATOM	1240	HB	VAL	128	105.612	100.748	90.316	1.00	0.00	H
ATOM	1241	1HG1	VAL	128	107.653	100.079	88.969	1.00	0.00	H
ATOM	1242	2HG1	VAL	128	108.447	99.557	90.475	1.00	0.00	H
ATOM	1243	3HG1	VAL	128	106.997	98.722	89.899	1.00	0.00	H
ATOM	1244	2HG2	VAL	128	105.597	100.584	92.771	1.00	0.00	H
ATOM	1245	3HG2	VAL	128	106.020	98.990	92.117	1.00	0.00	H
ATOM	1246	1HG2	VAL	128	107.283	100.036	92.811	1.00	0.00	H
ATOM	1247	N	VAL	129	108.436	103.608	89.266	0.00	0.00	N
ATOM	1248	CA	VAL	129	108.635	104.444	88.036	0.00	0.00	C
ATOM	1249	C	VAL	129	109.469	103.667	86.957	0.00	0.00	C
ATOM	1250	O	VAL	129	110.682	103.484	87.095	0.00	0.00	O
ATOM	1251	CB	VAL	129	109.234	105.842	88.417	0.00	0.00	C
ATOM	1252	CG1	VAL	129	109.436	106.777	87.201	0.00	0.00	C
ATOM	1253	CG2	VAL	129	108.356	106.644	89.410	0.00	0.00	C
ATOM	1254	H	VAL	129	109.032	103.732	90.098	0.00	0.00	H
ATOM	1255	HA	VAL	129	107.648	104.677	87.586	0.00	0.00	H
ATOM	1256	HB	VAL	129	110.228	105.683	88.887	0.00	0.00	H
ATOM	1257	1HG1	VAL	129	109.949	107.717	87.483	0.00	0.00	H
ATOM	1258	2HG1	VAL	129	110.064	106.319	86.415	0.00	0.00	H
ATOM	1259	3HG1	VAL	129	108.480	107.059	86.723	0.00	0.00	H
ATOM	1260	1HG2	VAL	129	108.744	107.665	89.571	0.00	0.00	H
ATOM	1261	2HG2	VAL	129	107.313	106.749	89.057	0.00	0.00	H
ATOM	1262	3HG2	VAL	129	108.321	106.161	90.404	0.00	0.00	H
ATOM	1263	N	LEU	130	108.799	103.224	85.886	1.00	0.00	N
ATOM	1264	CA	LEU	130	109.415	102.478	84.746	1.00	0.00	C
ATOM	1265	C	LEU	130	109.327	103.300	83.403	1.00	0.00	C
ATOM	1266	O	LEU	130	108.558	104.257	83.303	1.00	0.00	O
ATOM	1267	CB	LEU	130	108.620	101.133	84.676	1.00	0.00	C
ATOM	1268	CG	LEU	130	108.913	100.080	85.784	1.00	0.00	C
ATOM	1269	CD1	LEU	130	107.776	99.055	85.901	1.00	0.00	C
ATOM	1270	CD2	LEU	130	110.226	99.320	85.529	1.00	0.00	C
ATOM	1271	H	LEU	130	107.802	103.474	85.837	1.00	0.00	H
ATOM	1272	HA	LEU	130	110.488	102.267	84.925	1.00	0.00	H
ATOM	1273	1HB	LEU	130	107.535	101.361	84.647	1.00	0.00	H
ATOM	1274	2HB	LEU	130	108.787	100.665	83.694	1.00	0.00	H
ATOM	1275	HG	LEU	130	108.983	100.603	86.758	1.00	0.00	H
ATOM	1276	2HD1	LEU	130	107.947	98.341	86.729	1.00	0.00	H
ATOM	1277	3HD1	LEU	130	106.801	99.541	86.090	1.00	0.00	H
ATOM	1278	1HD1	LEU	130	107.665	98.457	84.978	1.00	0.00	H
ATOM	1279	2HD2	LEU	130	110.487	98.655	86.372	1.00	0.00	H
ATOM	1280	3HD2	LEU	130	110.172	99.585	84.626	1.00	0.00	H

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ATOM   1292  HA  GLU   131     110.247 104.702  81.185  0.00  0.00           H
ATOM   1293 1HB  GLU   131     111.036 103.469  79.097  0.00  0.00           H
ATOM   1294 2HB  GLU   131     111.040 101.969  79.995  0.00  0.00           H
ATOM   1295 1HG  GLU   131     112.861 102.929  81.533  0.00  0.00           H
ATOM   1296 2HG  GLU   131     112.727 104.481  80.717  0.00  0.00           H
ATOM   1297  N   LEU   132     108.277 104.581  79.443  1.00  0.00           N
ATOM   1298  CA  LEU   132     106.903 104.705  78.848  1.00  0.00           C
ATOM   1299  C   LEU   132     106.653 103.852  77.552  1.00  0.00           C
ATOM   1300  O   LEU   132     106.574 104.373  76.440  1.00  0.00           O
ATOM   1301  CB  LEU   132     106.596 106.229  78.718  1.00  0.00           C
ATOM   1302  CG  LEU   132     105.145 106.739  78.479  1.00  0.00           C
ATOM   1303  CD1 LEU   132     104.708 106.724  77.008  1.00  0.00           C
ATOM   1304  CD2 LEU   132     104.071 106.043  79.333  1.00  0.00           C
ATOM   1305  H   LEU   132     109.018 105.267  79.254  1.00  0.00           H
ATOM   1306  HA  LEU   132     106.180 104.329  79.594  1.00  0.00           H
ATOM   1307 1HB  LEU   132     106.924 106.718  79.651  1.00  0.00           H
ATOM   1308 2HB  LEU   132     107.268 106.664  77.950  1.00  0.00           H
ATOM   1309  HG  LEU   132     105.158 107.808  78.772  1.00  0.00           H
ATOM   1310 2HD1 LEU   132     103.786 107.316  76.851  1.00  0.00           H
ATOM   1311 3HD1 LEU   132     105.484 107.156  76.347  1.00  0.00           H
ATOM   1312 1HD1 LEU   132     104.505 105.704  76.637  1.00  0.00           H
ATOM   1313 2HD2 LEU   132     103.075 106.495  79.174  1.00  0.00           H
ATOM   1314 3HD2 LEU   132     103.980 104.969  79.087  1.00  0.00           H
ATOM   1315 1HD2 LEU   132     104.296 106.123  80.410  1.00  0.00           H
ATOM   1316  N   CYS   133     106.472 102.527  77.702  1.00  0.00           N
ATOM   1317  CA  CYS   133     106.426 101.589  76.542  1.00  0.00           C
ATOM   1318  C   CYS   133     105.037 100.892  76.285  1.00  0.00           C
ATOM   1319  O   CYS   133     104.198 100.720  77.177  1.00  0.00           O
ATOM   1320  CB  CYS   133     107.598 100.603  76.742  1.00  0.00           C
ATOM   1321  SG  CYS   133     109.201 101.492  76.858  1.00  0.00           S
ATOM   1322  H   CYS   133     106.732 102.222  78.648  1.00  0.00           H
ATOM   1323  HA  CYS   133     106.666 102.141  75.607  1.00  0.00           H
ATOM   1324 1HB  CYS   133     107.458  99.988  77.648  1.00  0.00           H
ATOM   1325 2HB  CYS   133     107.663  99.900  75.893  1.00  0.00           H
ATOM   1326  HG  CYS   133     109.042 102.358  75.852  1.00  0.00           H
ATOM   1327  N   ARG   134     104.775 100.465  75.033  1.00  0.00           N
ATOM   1328  CA  ARG   134     103.490  99.798  74.659  1.00  0.00           C
ATOM   1329  C   ARG   134     103.590  98.225  74.735  1.00  0.00           C
ATOM   1330  O   ARG   134     104.065  97.571  73.813  1.00  0.00           O
ATOM   1331  CB  ARG   134     103.084 100.221  73.216  1.00  0.00           C
ATOM   1332  CG  ARG   134     102.443 101.619  73.038  1.00  0.00           C
ATOM   1333  CD  ARG   134     101.887 101.772  71.607  1.00  0.00           C
ATOM   1334  NE  ARG   134     101.161 103.064  71.452  1.00  0.00           N
ATOM   1335  CZ  ARG   134     100.461 103.419  70.376  1.00  0.00           C
ATOM   1336  NH1 ARG   134     100.385 102.699  69.293  1.00  0.00           N
ATOM   1337  NH2 ARG   134      99.837 104.556  70.389  1.00  0.00           N
ATOM   1338  HE  ARG   134     101.171 103.752  72.213  1.00  0.00           H
ATOM   1339  H   ARG   134     105.593 100.514  74.405  1.00  0.00           H
ATOM   1340  HA  ARG   134     102.674 100.125  75.335  1.00  0.00           H
ATOM   1341 1HB  ARG   134     103.960 100.113  72.542  1.00  0.00           H
ATOM   1342 2HB  ARG   134     102.359  99.472  72.836  1.00  0.00           H
ATOM   1343 1HG  ARG   134     101.637 101.756  73.785  1.00  0.00           H
ATOM   1344 2HG  ARG   134     103.197 102.403  73.263  1.00  0.00           H
ATOM   1345 1HD  ARG   134     102.727 101.701  70.882  1.00  0.00           H
ATOM   1346 2HD  ARG   134     101.205 100.921  71.383  1.00  0.00           H
ATOM   1347 2HH1 ARG   134     100.927 101.836  69.356  1.00  0.00           H
ATOM   1348 1HH1 ARG   134      99.983 103.155  68.477  1.00  0.00           H
ATOM   1349 1HH2 ARG   134      99.920 105.082  71.261  1.00  0.00           H
ATOM   1350 2HH2 ARG   134      99.221 104.761  69.596  1.00  0.00           H
ATOM   1351  N   ARG   135     103.087  97.624  75.813  1.00  0.00           N
ATOM   1352  CA  ARG   135     102.444  96.259  75.882  1.00  0.00           C
ATOM   1353  C   ARG   135     102.227  95.298  74.626  1.00  0.00           C
ATOM   1354  O   ARG   135     102.193  95.768  73.496  1.00  0.00           O
ATOM   1355  CB  ARG   135     101.170  96.500  76.763  1.00  0.00           C
ATOM   1356  CG  ARG   135     100.249  97.756  76.533  1.00  0.00           C
ATOM   1357  CD  ARG   135      99.239  98.054  77.662  1.00  0.00           C
ATOM   1358  NE  ARG   135      98.236  96.968  77.722  1.00  0.00           N
ATOM   1359  CZ  ARG   135      98.273  96.032  78.641  1.00  0.00           C
ATOM   1360  NH1 ARG   135      98.483  96.230  79.894  1.00  0.00           N
ATOM   1361  NH2 ARG   135      98.048  94.829  78.294  1.00  0.00           N
ATOM   1362  HE  ARG   135      97.982  96.480  76.853  1.00  0.00           H
ATOM   1363  H   ARG   135     102.981  98.280  76.595  1.00  0.00           H
ATOM   1364  HA  ARG   135     103.127  95.662  76.520  1.00  0.00           H
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ATOM	1365	1HB	ARG	135	100.547	95.585	76.749	1.00	0.00	H
ATOM	1366	2HB	ARG	135	101.503	96.524	77.819	1.00	0.00	H
ATOM	1367	1HG	ARG	135	100.861	98.670	76.445	1.00	0.00	H
ATOM	1368	2HG	ARG	135	99.741	97.682	75.554	1.00	0.00	H
ATOM	1369	1HD	ARG	135	99.775	98.187	78.627	1.00	0.00	H
ATOM	1370	2HD	ARG	135	98.722	99.018	77.487	1.00	0.00	H
ATOM	1371	2HH1	ARG	135	97.841	96.966	80.275	1.00	0.00	H
ATOM	1372	1HH1	ARG	135	98.325	95.288	80.351	1.00	0.00	H
ATOM	1373	1HH2	ARG	135	97.606	94.599	77.401	1.00	0.00	H
ATOM	1374	2HH2	ARG	135	97.832	94.231	79.153	1.00	0.00	H
ATOM	1375	N	ARG	136	102.093	93.951	74.777	1.00	0.00	N
ATOM	1376	CA	ARG	136	102.057	92.967	73.624	1.00	0.00	C
ATOM	1377	C	ARG	136	100.688	92.376	73.061	1.00	0.00	C
ATOM	1378	O	ARG	136	100.739	91.506	72.193	1.00	0.00	O
ATOM	1379	CB	ARG	136	103.087	91.811	73.900	1.00	0.00	C
ATOM	1380	CG	ARG	136	104.158	91.580	72.810	1.00	0.00	C
ATOM	1381	CD	ARG	136	105.251	92.657	72.832	1.00	0.00	C
ATOM	1382	NE	ARG	136	106.206	92.383	71.732	1.00	0.00	N
ATOM	1383	CZ	ARG	136	107.389	92.960	71.582	1.00	0.00	C
ATOM	1384	NH1	ARG	136	107.878	93.831	72.403	1.00	0.00	N
ATOM	1385	NH2	ARG	136	108.094	92.643	70.557	1.00	0.00	N
ATOM	1386	HE	ARG	136	105.927	91.687	71.026	1.00	0.00	H
ATOM	1387	H	ARG	136	102.248	93.616	75.740	1.00	0.00	H
ATOM	1388	HA	ARG	136	102.443	93.480	72.718	1.00	0.00	H
ATOM	1389	1HB	ARG	136	103.582	91.925	74.880	1.00	0.00	H
ATOM	1390	2HB	ARG	136	102.546	90.859	74.040	1.00	0.00	H
ATOM	1391	1HG	ARG	136	104.633	90.591	72.959	1.00	0.00	H
ATOM	1392	2HG	ARG	136	103.686	91.522	71.809	1.00	0.00	H
ATOM	1393	1HD	ARG	136	104.817	93.671	72.717	1.00	0.00	H
ATOM	1394	2HD	ARG	136	105.766	92.652	73.815	1.00	0.00	H
ATOM	1395	2HH1	ARG	136	107.240	94.080	73.160	1.00	0.00	H
ATOM	1396	1HH1	ARG	136	108.786	94.233	72.170	1.00	0.00	H
ATOM	1397	1HH2	ARG	136	107.610	91.983	69.942	1.00	0.00	H
ATOM	1398	2HH2	ARG	136	108.989	93.111	70.433	1.00	0.00	H
ATOM	1399	N	SER	137	99.408	92.748	73.311	1.00	0.00	N
ATOM	1400	CA	SER	137	98.894	93.583	74.450	1.00	0.00	C
ATOM	1401	C	SER	137	98.599	95.136	74.259	1.00	0.00	C
ATOM	1402	O	SER	137	98.196	95.769	75.225	1.00	0.00	O
ATOM	1403	CB	SER	137	97.668	92.796	75.047	1.00	0.00	C
ATOM	1404	OG	SER	137	96.959	93.495	76.093	1.00	0.00	O
ATOM	1405	H	SER	137	98.778	92.393	72.582	1.00	0.00	H
ATOM	1406	HA	SER	137	99.623	93.559	75.279	1.00	0.00	H
ATOM	1407	1HB	SER	137	96.937	92.555	74.252	1.00	0.00	H
ATOM	1408	2HB	SER	137	97.996	91.822	75.453	1.00	0.00	H
ATOM	1409	HG	SER	137	96.783	92.949	76.949	1.00	0.00	H
ATOM	1410	N	LEU	138	98.732	96.006	73.240	1.00	0.00	N
ATOM	1411	CA	LEU	138	98.781	95.723	71.777	1.00	0.00	C
ATOM	1412	C	LEU	138	97.517	94.909	71.295	1.00	0.00	C
ATOM	1413	O	LEU	138	97.528	93.692	71.106	1.00	0.00	O
ATOM	1414	CB	LEU	138	100.246	95.409	71.362	1.00	0.00	C
ATOM	1415	CG	LEU	138	100.687	95.099	69.916	1.00	0.00	C
ATOM	1416	CD1	LEU	138	102.198	94.813	69.905	1.00	0.00	C
ATOM	1417	CD2	LEU	138	100.015	93.877	69.283	1.00	0.00	C
ATOM	1418	H	LEU	138	98.550	96.940	73.620	1.00	0.00	H
ATOM	1419	HA	LEU	138	98.653	96.705	71.281	1.00	0.00	H
ATOM	1420	1HB	LEU	138	100.846	96.286	71.679	1.00	0.00	H
ATOM	1421	2HB	LEU	138	100.635	94.628	72.003	1.00	0.00	H
ATOM	1422	HG	LEU	138	100.492	95.999	69.305	1.00	0.00	H
ATOM	1423	2HD1	LEU	138	102.762	95.565	70.484	1.00	0.00	H
ATOM	1424	3HD1	LEU	138	102.447	93.835	70.362	1.00	0.00	H
ATOM	1425	1HD1	LEU	138	102.610	94.806	68.881	1.00	0.00	H
ATOM	1426	2HD2	LEU	138	100.062	92.841	69.350	1.00	0.00	H
ATOM	1427	3HD2	LEU	138	99.315	93.053	69.012	1.00	0.00	H

ATOM	1438	HA	LEU	139	95.105	94.027	70.683	1.00	0.00	H
ATOM	1439	1HB	LEU	139	95.156	95.360	73.209	1.00	0.00	H
ATOM	1440	2HB	LEU	139	93.707	96.006	72.523	1.00	0.00	H
ATOM	1441	HG	LEU	139	94.301	92.982	72.746	1.00	0.00	H
ATOM	1442	2HD1	LEU	139	94.379	94.064	75.041	1.00	0.00	H
ATOM	1443	3HD1	LEU	139	92.776	94.796	74.746	1.00	0.00	H
ATOM	1444	1HD1	LEU	139	92.958	93.031	74.876	1.00	0.00	H
ATOM	1445	2HD2	LEU	139	91.625	94.498	72.380	1.00	0.00	H
ATOM	1446	3HD2	LEU	139	92.420	93.425	71.210	1.00	0.00	H
ATOM	1447	1HD2	LEU	139	91.766	92.749	72.704	1.00	0.00	H
ATOM	1448	N	GLU	140	94.311	96.661	68.919	1.00	0.00	N
ATOM	1449	CA	GLU	140	95.583	97.311	68.479	1.00	0.00	C
ATOM	1450	C	GLU	140	96.622	96.377	67.752	1.00	0.00	C
ATOM	1451	O	GLU	140	96.907	95.279	68.222	1.00	0.00	O
ATOM	1452	CB	GLU	140	96.197	98.284	69.534	1.00	0.00	C
ATOM	1453	CG	GLU	140	96.556	99.716	69.056	1.00	0.00	C
ATOM	1454	CD	GLU	140	97.614	100.407	69.926	1.00	0.00	C
ATOM	1455	OE1	GLU	140	98.716	99.888	70.184	1.00	0.00	O
ATOM	1456	OE2	GLU	140	97.295	101.695	70.221	1.00	0.00	O
ATOM	1457	H	GLU	140	93.439	96.792	68.391	1.00	0.00	H
ATOM	1458	HA	GLU	140	95.204	97.973	67.674	1.00	0.00	H
ATOM	1459	1HB	GLU	140	95.535	98.373	70.417	1.00	0.00	H
ATOM	1460	2HB	GLU	140	97.116	97.812	69.926	1.00	0.00	H
ATOM	1461	1HG	GLU	140	96.948	99.703	68.025	1.00	0.00	H
ATOM	1462	2HG	GLU	140	95.644	100.338	69.008	1.00	0.00	H
ATOM	1463	N	LEU	141	97.189	96.813	66.605	1.00	0.00	N
ATOM	1464	CA	LEU	141	98.215	96.059	65.806	1.00	0.00	C
ATOM	1465	C	LEU	141	97.869	94.561	65.465	1.00	0.00	C
ATOM	1466	O	LEU	141	97.231	94.319	64.446	1.00	0.00	O
ATOM	1467	CB	LEU	141	99.684	96.288	66.287	1.00	0.00	C
ATOM	1468	CG	LEU	141	100.294	97.716	66.239	1.00	0.00	C
ATOM	1469	CD1	LEU	141	99.949	98.559	67.478	1.00	0.00	C
ATOM	1470	CD2	LEU	141	101.828	97.644	66.150	1.00	0.00	C
ATOM	1471	H	LEU	141	96.894	97.753	66.330	1.00	0.00	H
ATOM	1472	HA	LEU	141	98.193	96.531	64.805	1.00	0.00	H
ATOM	1473	1HB	LEU	141	99.800	95.860	67.293	1.00	0.00	H
ATOM	1474	2HB	LEU	141	100.316	95.635	65.650	1.00	0.00	H
ATOM	1475	HG	LEU	141	99.924	98.234	65.331	1.00	0.00	H
ATOM	1476	2HD1	LEU	141	98.865	98.650	67.627	1.00	0.00	H
ATOM	1477	3HD1	LEU	141	100.359	98.128	68.411	1.00	0.00	H
ATOM	1478	1HD1	LEU	141	100.344	99.590	67.401	1.00	0.00	H
ATOM	1479	2HD2	LEU	141	102.277	97.137	67.025	1.00	0.00	H
ATOM	1480	3HD2	LEU	141	102.157	97.089	65.253	1.00	0.00	H
ATOM	1481	1HD2	LEU	141	102.288	98.647	66.082	1.00	0.00	H
ATOM	1482	N	HIS	142	98.239	93.574	66.305	1.00	0.00	N
ATOM	1483	CA	HIS	142	97.890	92.130	66.120	1.00	0.00	C
ATOM	1484	C	HIS	142	96.376	91.786	65.867	1.00	0.00	C
ATOM	1485	O	HIS	142	96.077	91.082	64.902	1.00	0.00	O
ATOM	1486	CB	HIS	142	98.520	91.384	67.333	1.00	0.00	C
ATOM	1487	CG	HIS	142	98.401	89.863	67.314	1.00	0.00	C
ATOM	1488	ND1	HIS	142	99.032	89.064	66.378	1.00	0.00	N
ATOM	1489	CE1	HIS	142	98.517	87.850	66.743	1.00	0.00	C
ATOM	1490	NE2	HIS	142	97.673	87.762	67.818	1.00	0.00	N
ATOM	1491	CD2	HIS	142	97.591	89.095	68.166	1.00	0.00	C
ATOM	1492	H	HIS	142	98.568	93.935	67.207	1.00	0.00	H
ATOM	1493	HA	HIS	142	98.425	91.776	65.215	1.00	0.00	H
ATOM	1494	1HB	HIS	142	99.601	91.610	67.390	1.00	0.00	H
ATOM	1495	2HB	HIS	142	98.095	91.771	68.280	1.00	0.00	H
ATOM	1496	HE1	HIS	142	98.758	86.968	66.161	1.00	0.00	H
ATOM	1497	HE2	HIS	142	97.139	86.941	68.140	1.00	0.00	H
ATOM	1498	HD2	HIS	142	96.957	89.499	68.943	1.00	0.00	H
ATOM	1499	N	LYS	143	95.427	92.296	66.675	1.00	0.00	N
ATOM	1500	CA	LYS	143	93.966	92.168	66.366	1.00	0.00	C
ATOM	1501	C	LYS	143	93.456	92.911	65.071	1.00	0.00	C
ATOM	1502	O	LYS	143	92.547	92.416	64.401	1.00	0.00	O
ATOM	1503	CB	LYS	143	93.182	92.544	67.652	1.00	0.00	C
ATOM	1504	CG	LYS	143	91.694	92.119	67.639	1.00	0.00	C
ATOM	1505	CD	LYS	143	90.996	92.400	68.981	1.00	0.00	C
ATOM	1506	CE	LYS	143	89.522	91.976	68.981	1.00	0.00	C
ATOM	1507	NZ	LYS	143	88.936	92.262	70.305	1.00	0.00	N
ATOM	1508	1HZ	LYS	143	87.946	91.979	70.312	1.00	0.00	H
ATOM	1509	2HZ	LYS	143	89.448	91.737	71.029	1.00	0.00	H
ATOM	1510	3HZ	LYS	143	89.005	93.271	70.501	1.00	0.00	H

ATOM	1511	H	LYS	143	95.796	92.914	67.405	1.00	0.00	H
ATOM	1512	HA	LYS	143	93.768	91.094	66.174	1.00	0.00	H
ATOM	1513	1HB	LYS	143	93.663	92.071	68.532	1.00	0.00	H
ATOM	1514	2HB	LYS	143	93.260	93.634	67.831	1.00	0.00	H
ATOM	1515	1HG	LYS	143	91.157	92.643	66.822	1.00	0.00	H
ATOM	1516	2HG	LYS	143	91.612	91.041	67.399	1.00	0.00	H
ATOM	1517	1HD	LYS	143	91.533	91.864	69.788	1.00	0.00	H
ATOM	1518	2HD	LYS	143	91.083	93.480	69.220	1.00	0.00	H
ATOM	1519	1HE	LYS	143	88.963	92.511	68.187	1.00	0.00	H
ATOM	1520	2HE	LYS	143	89.428	90.895	68.753	1.00	0.00	H
ATOM	1521	N	ARG	144	94.052	94.055	64.693	0.00	0.00	N
ATOM	1522	CA	ARG	144	93.818	94.707	63.364	0.00	0.00	C
ATOM	1523	C	ARG	144	94.430	93.932	62.133	0.00	0.00	C
ATOM	1524	O	ARG	144	93.771	93.765	61.107	0.00	0.00	O
ATOM	1525	CB	ARG	144	94.325	96.187	63.398	0.00	0.00	C
ATOM	1526	CG	ARG	144	94.048	97.079	64.638	0.00	0.00	C
ATOM	1527	CD	ARG	144	92.575	97.236	65.036	0.00	0.00	C
ATOM	1528	NE	ARG	144	92.517	98.058	66.275	0.00	0.00	N
ATOM	1529	CZ	ARG	144	91.428	98.276	67.001	0.00	0.00	C
ATOM	1530	NH1	ARG	144	90.254	97.796	66.722	0.00	0.00	N
ATOM	1531	NH2	ARG	144	91.551	99.010	68.049	0.00	0.00	N
ATOM	1532	HE	ARG	144	93.394	98.494	66.595	1.00	0.00	H
ATOM	1533	H	ARG	144	94.877	94.270	65.261	0.00	0.00	H
ATOM	1534	HA	ARG	144	92.724	94.742	63.188	0.00	0.00	H
ATOM	1535	1HB	ARG	144	93.934	96.702	62.499	0.00	0.00	H
ATOM	1536	2HB	ARG	144	95.422	96.182	63.249	0.00	0.00	H
ATOM	1537	1HG	ARG	144	94.490	98.081	64.473	0.00	0.00	H
ATOM	1538	2HG	ARG	144	94.603	96.661	65.499	0.00	0.00	H
ATOM	1539	1HD	ARG	144	92.121	96.238	65.209	0.00	0.00	H
ATOM	1540	2HD	ARG	144	91.997	97.713	64.219	0.00	0.00	H
ATOM	1541	1HH1	ARG	144	89.492	98.028	67.359	0.00	0.00	H
ATOM	1542	2HH1	ARG	144	90.243	97.220	65.880	0.00	0.00	H
ATOM	1543	1HH2	ARG	144	90.714	99.175	68.606	0.00	0.00	H
ATOM	1544	2HH2	ARG	144	92.504	99.350	68.179	0.00	0.00	H
ATOM	1545	N	ARG	145	95.685	93.464	62.247	1.00	0.00	N
ATOM	1546	CA	ARG	145	96.370	92.597	61.243	1.00	0.00	C
ATOM	1547	C	ARG	145	95.872	91.111	61.094	1.00	0.00	C
ATOM	1548	O	ARG	145	96.228	90.473	60.101	1.00	0.00	O
ATOM	1549	CB	ARG	145	97.877	92.563	61.650	1.00	0.00	C
ATOM	1550	CG	ARG	145	98.679	93.889	61.575	1.00	0.00	C
ATOM	1551	CD	ARG	145	100.051	93.757	62.256	1.00	0.00	C
ATOM	1552	NE	ARG	145	100.752	95.066	62.215	1.00	0.00	N
ATOM	1553	CZ	ARG	145	102.002	95.278	62.604	1.00	0.00	C
ATOM	1554	NH1	ARG	145	102.785	94.365	63.098	1.00	0.00	N
ATOM	1555	NH2	ARG	145	102.465	96.470	62.475	1.00	0.00	N
ATOM	1556	HE	ARG	145	100.224	95.874	61.856	1.00	0.00	H
ATOM	1557	H	ARG	145	96.135	93.688	63.146	1.00	0.00	H
ATOM	1558	HA	ARG	145	96.281	93.057	60.240	1.00	0.00	H
ATOM	1559	1HB	ARG	145	97.951	92.141	62.674	1.00	0.00	H
ATOM	1560	2HB	ARG	145	98.410	91.821	61.021	1.00	0.00	H
ATOM	1561	1HG	ARG	145	98.805	94.204	60.520	1.00	0.00	H
ATOM	1562	2HG	ARG	145	98.115	94.711	62.056	1.00	0.00	H
ATOM	1563	1HD	ARG	145	99.923	93.427	63.309	1.00	0.00	H
ATOM	1564	2HD	ARG	145	100.648	92.971	61.751	1.00	0.00	H
ATOM	1565	2HH1	ARG	145	102.341	93.449	63.156	1.00	0.00	H
ATOM	1566	1HH1	ARG	145	103.735	94.640	63.347	1.00	0.00	H
ATOM	1567	1HH2	ARG	145	101.776	97.099	62.057	1.00	0.00	H
ATOM	1568	2HH2	ARG	145	103.434	96.635	62.741	1.00	0.00	H
ATOM	1569	N	LYS	146	95.154	90.529	62.082	1.00	0.00	N
ATOM	1570	CA	LYS	146	94.909	89.056	63.315	1.00	0.00	C
ATOM	1571	C	LYS	146	96.148	88.227	62.721	1.00	0.00	C
ATOM	1572	O	LYS	146	96.378	87.587	63.775	1.00	0.00	C
ATOM	1573	CB	LYS	146	94.153	88.153	62.333	1.00	0.00	C

ATOM	1584	2HB	LYS	146	94.824	88.464	60.112	1.00	0.00	H
ATOM	1585	1HG	LYS	146	94.419	86.340	61.489	1.00	0.00	H
ATOM	1586	2HG	LYS	146	92.866	87.000	62.003	1.00	0.00	H
ATOM	1587	1HD	LYS	146	92.118	87.145	59.582	1.00	0.00	H
ATOM	1588	2HD	LYS	146	93.694	86.549	59.054	1.00	0.00	H
ATOM	1589	1HE	LYS	146	93.296	84.375	60.333	1.00	0.00	H
ATOM	1590	2HE	LYS	146	91.704	84.972	60.836	1.00	0.00	H
ATOM	1591	N	ALA	147	97.248	88.196	61.950	1.00	0.00	N
ATOM	1592	CA	ALA	147	98.402	87.294	62.187	1.00	0.00	C
ATOM	1593	C	ALA	147	99.779	87.983	61.895	1.00	0.00	C
ATOM	1594	O	ALA	147	99.933	88.722	60.915	1.00	0.00	O
ATOM	1595	CB	ALA	147	98.170	86.085	61.256	1.00	0.00	C
ATOM	1596	H	ALA	147	97.178	88.800	61.122	1.00	0.00	H
ATOM	1597	HA	ALA	147	98.408	86.934	63.237	1.00	0.00	H
ATOM	1598	2HB	ALA	147	97.255	85.528	61.536	1.00	0.00	H
ATOM	1599	3HB	ALA	147	98.071	86.380	60.195	1.00	0.00	H
ATOM	1600	1HB	ALA	147	99.006	85.368	61.308	1.00	0.00	H
ATOM	1601	N	LEU	148	100.806	87.700	62.716	1.00	0.00	N
ATOM	1602	CA	LEU	148	102.207	88.129	62.439	1.00	0.00	C
ATOM	1603	C	LEU	148	102.986	87.003	61.680	1.00	0.00	C
ATOM	1604	O	LEU	148	103.014	85.843	62.105	1.00	0.00	O
ATOM	1605	CB	LEU	148	102.939	88.519	63.757	1.00	0.00	C
ATOM	1606	CG	LEU	148	102.326	89.637	64.641	1.00	0.00	C
ATOM	1607	CD1	LEU	148	103.212	89.891	65.868	1.00	0.00	C
ATOM	1608	CD2	LEU	148	102.098	90.967	63.907	1.00	0.00	C
ATOM	1609	H	LEU	148	100.590	87.057	63.490	1.00	0.00	H
ATOM	1610	HA	LEU	148	102.200	89.037	61.803	1.00	0.00	H
ATOM	1611	1HB	LEU	148	103.042	87.607	64.378	1.00	0.00	H
ATOM	1612	2HB	LEU	148	103.981	88.795	63.509	1.00	0.00	H
ATOM	1613	HG	LEU	148	101.343	89.275	65.004	1.00	0.00	H
ATOM	1614	2HD1	LEU	148	103.436	88.954	66.407	1.00	0.00	H
ATOM	1615	3HD1	LEU	148	104.185	90.351	65.609	1.00	0.00	H
ATOM	1616	1HD1	LEU	148	102.720	90.564	66.595	1.00	0.00	H
ATOM	1617	2HD2	LEU	148	103.034	91.381	63.491	1.00	0.00	H
ATOM	1618	3HD2	LEU	148	101.382	90.848	63.072	1.00	0.00	H
ATOM	1619	1HD2	LEU	148	101.664	91.730	64.580	1.00	0.00	H
ATOM	1620	N	THR	149	103.648	87.338	60.563	1.00	0.00	N
ATOM	1621	CA	THR	149	104.435	86.350	59.754	1.00	0.00	C
ATOM	1622	C	THR	149	105.682	85.746	60.498	1.00	0.00	C
ATOM	1623	O	THR	149	106.190	86.324	61.461	1.00	0.00	O
ATOM	1624	CB	THR	149	104.837	86.961	58.370	1.00	0.00	C
ATOM	1625	OG1	THR	149	105.679	88.098	58.524	1.00	0.00	O
ATOM	1626	CG2	THR	149	103.673	87.383	57.459	1.00	0.00	C
ATOM	1627	H	THR	149	103.553	88.318	60.285	1.00	0.00	H
ATOM	1628	HA	THR	149	103.758	85.496	59.545	1.00	0.00	H
ATOM	1629	HB	THR	149	105.407	86.192	57.810	1.00	0.00	H
ATOM	1630	HG1	THR	149	105.422	88.711	57.831	1.00	0.00	H
ATOM	1631	1HG2	THR	149	104.024	87.738	56.472	1.00	0.00	H
ATOM	1632	2HG2	THR	149	102.982	86.539	57.266	1.00	0.00	H
ATOM	1633	3HG2	THR	149	103.065	88.194	57.904	1.00	0.00	H
ATOM	1634	N	GLU	150	106.193	84.586	60.038	0.00	0.00	N
ATOM	1635	CA	GLU	150	107.355	83.885	60.680	0.00	0.00	C
ATOM	1636	C	GLU	150	108.671	84.748	60.925	0.00	0.00	C
ATOM	1637	O	GLU	150	109.164	84.675	62.052	0.00	0.00	O
ATOM	1638	CB	GLU	150	107.587	82.517	59.960	0.00	0.00	C
ATOM	1639	CG	GLU	150	106.402	81.503	60.039	0.00	0.00	C
ATOM	1640	CD	GLU	150	106.509	80.210	59.224	0.00	0.00	C
ATOM	1641	OE1	GLU	150	107.099	79.207	59.610	0.00	0.00	O
ATOM	1642	OE2	GLU	150	105.835	80.283	58.040	0.00	0.00	O
ATOM	1643	H	GLU	150	105.612	84.128	59.330	0.00	0.00	H
ATOM	1644	HA	GLU	150	107.022	83.624	61.706	0.00	0.00	H
ATOM	1645	1HB	GLU	150	108.487	82.034	60.389	0.00	0.00	H
ATOM	1646	2HB	GLU	150	107.856	82.703	58.907	0.00	0.00	H
ATOM	1647	1HG	GLU	150	105.461	81.993	59.736	0.00	0.00	H
ATOM	1648	2HG	GLU	150	106.235	81.212	61.092	0.00	0.00	H
ATOM	1649	N	PRO	151	109.214	85.621	60.014	0.00	0.00	N
ATOM	1650	CA	PRO	151	110.199	86.694	60.384	0.00	0.00	C
ATOM	1651	CD	PRO	151	108.872	85.617	58.583	0.00	0.00	C
ATOM	1652	C	PRO	151	109.855	87.723	61.524	0.00	0.00	C
ATOM	1653	O	PRO	151	110.743	88.145	62.266	0.00	0.00	O
ATOM	1654	CB	PRO	151	110.413	87.422	59.037	0.00	0.00	C
ATOM	1655	CG	PRO	151	109.986	86.440	57.949	0.00	0.00	C
ATOM	1656	HA	PRO	151	111.150	86.203	60.668	0.00	0.00	H

ATOM	1657	1HD	PRO	151	107.885	86.088	58.412	0.00	0.00	H
ATOM	1658	2HD	PRO	151	108.856	84.598	58.157	0.00	0.00	H
ATOM	1659	1HB	PRO	151	111.462	87.754	58.917	0.00	0.00	H
ATOM	1660	2HB	PRO	151	109.787	88.335	58.968	0.00	0.00	H
ATOM	1661	1HG	PRO	151	110.834	85.785	57.690	0.00	0.00	H
ATOM	1662	2HG	PRO	151	109.669	86.944	57.018	0.00	0.00	H
ATOM	1663	N	GLU	152	108.587	88.146	61.648	1.00	0.00	N
ATOM	1664	CA	GLU	152	108.117	89.007	62.775	1.00	0.00	C
ATOM	1665	C	GLU	152	107.904	88.238	64.129	1.00	0.00	C
ATOM	1666	O	GLU	152	108.439	88.657	65.158	1.00	0.00	O
ATOM	1667	CB	GLU	152	106.855	89.756	62.250	1.00	0.00	C
ATOM	1668	CG	GLU	152	106.211	90.800	63.203	1.00	0.00	C
ATOM	1669	CD	GLU	152	106.987	92.086	63.492	1.00	0.00	C
ATOM	1670	OE1	GLU	152	108.200	92.220	63.370	1.00	0.00	O
ATOM	1671	OE2	GLU	152	106.172	93.078	63.939	1.00	0.00	O
ATOM	1672	H	GLU	152	107.932	87.605	61.072	1.00	0.00	H
ATOM	1673	HA	GLU	152	108.892	89.773	62.981	1.00	0.00	H
ATOM	1674	1HB	GLU	152	107.096	90.261	61.293	1.00	0.00	H
ATOM	1675	2HB	GLU	152	106.081	89.009	61.984	1.00	0.00	H
ATOM	1676	1HG	GLU	152	105.230	91.093	62.786	1.00	0.00	H
ATOM	1677	2HG	GLU	152	105.977	90.333	64.176	1.00	0.00	H
ATOM	1678	N	ALA	153	107.158	87.116	64.137	0.00	0.00	N
ATOM	1679	CA	ALA	153	107.037	86.226	65.325	0.00	0.00	C
ATOM	1680	C	ALA	153	108.359	85.596	65.902	0.00	0.00	C
ATOM	1681	O	ALA	153	108.492	85.516	67.125	0.00	0.00	O
ATOM	1682	CB	ALA	153	105.982	85.168	64.944	0.00	0.00	C
ATOM	1683	H	ALA	153	106.793	86.850	63.212	0.00	0.00	H
ATOM	1684	HA	ALA	153	106.608	86.829	66.151	0.00	0.00	H
ATOM	1685	1HB	ALA	153	105.751	84.502	65.795	0.00	0.00	H
ATOM	1686	2HB	ALA	153	105.021	85.624	64.636	0.00	0.00	H
ATOM	1687	3HB	ALA	153	106.317	84.525	64.108	0.00	0.00	H
ATOM	1688	N	ARG	154	109.343	85.199	65.066	0.00	0.00	N
ATOM	1689	CA	ARG	154	110.722	84.852	65.539	0.00	0.00	C
ATOM	1690	C	ARG	154	111.530	85.995	66.258	0.00	0.00	C
ATOM	1691	O	ARG	154	112.158	85.741	67.286	0.00	0.00	O
ATOM	1692	CB	ARG	154	111.503	84.146	64.390	0.00	0.00	C
ATOM	1693	CG	ARG	154	112.107	85.065	63.296	0.00	0.00	C
ATOM	1694	CD	ARG	154	113.543	85.528	63.593	0.00	0.00	C
ATOM	1695	NE	ARG	154	113.880	86.656	62.687	0.00	0.00	N
ATOM	1696	CZ	ARG	154	114.866	87.527	62.870	0.00	0.00	C
ATOM	1697	NH1	ARG	154	115.740	87.459	63.831	0.00	0.00	N
ATOM	1698	NH2	ARG	154	114.962	88.493	62.030	0.00	0.00	N
ATOM	1699	HE	ARG	154	113.299	86.772	61.844	1.00	0.00	H
ATOM	1700	H	ARG	154	109.127	85.334	64.069	0.00	0.00	H
ATOM	1701	HA	ARG	154	110.592	84.074	66.310	0.00	0.00	H
ATOM	1702	1HB	ARG	154	110.836	83.409	63.904	0.00	0.00	H
ATOM	1703	2HB	ARG	154	112.305	83.522	64.828	0.00	0.00	H
ATOM	1704	1HG	ARG	154	111.443	85.935	63.149	0.00	0.00	H
ATOM	1705	2HG	ARG	154	112.090	84.564	62.315	0.00	0.00	H
ATOM	1706	1HD	ARG	154	114.240	84.680	63.473	0.00	0.00	H
ATOM	1707	2HD	ARG	154	113.654	85.843	64.648	0.00	0.00	H
ATOM	1708	1HH1	ARG	154	116.480	88.160	63.838	0.00	0.00	H
ATOM	1709	2HH1	ARG	154	115.646	86.618	64.402	0.00	0.00	H
ATOM	1710	1HH2	ARG	154	115.697	89.181	62.187	0.00	0.00	H
ATOM	1711	2HH2	ARG	154	114.203	88.476	61.347	0.00	0.00	H
ATOM	1712	N	TYR	155	111.514	87.235	65.733	1.00	0.00	N
ATOM	1713	CA	TYR	155	112.066	88.440	66.422	1.00	0.00	C
ATOM	1714	C	TYR	155	111.457	88.734	67.843	1.00	0.00	C
ATOM	1715	O	TYR	155	112.186	89.051	68.784	1.00	0.00	O
ATOM	1716	CB	TYR	155	111.095	89.611	65.411	1.00	0.00	C
ATOM	1717	CG	TYR	155	112.698	90.878	65.739	1.00	0.00	C
ATOM	1718	CD1	TYR	155	113.0[illegible]	91.0[illegible]	67.[illegible]	1.00	0.00	C

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ATOM   1730  HE1 TYR   155     115.698  92.323  65.073  1.00  0.00           H
ATOM   1731  HE2 TYR   155     112.486  93.787  67.484  1.00  0.00           H
ATOM   1732  HH  TYR   155     114.330  94.967  66.971  1.00  0.00           H
ATOM   1733  N   TYR   156     110.132  88.574  67.992  0.00  0.00           N
ATOM   1734  CA  TYR   156     109.433  88.599  69.304  0.00  0.00           C
ATOM   1735  C   TYR   156     109.852  87.428  70.275  0.00  0.00           C
ATOM   1736  O   TYR   156     110.195  87.710  71.422  0.00  0.00           O
ATOM   1737  CB  TYR   156     107.898  88.642  69.018  0.00  0.00           C
ATOM   1738  CG  TYR   156     107.223  89.943  68.497  0.00  0.00           C
ATOM   1739  CD1 TYR   156     107.798  90.774  67.520  0.00  0.00           C
ATOM   1740  CE1 TYR   156     107.141  91.923  67.090  0.00  0.00           C
ATOM   1741  CZ  TYR   156     105.895  92.247  67.606  0.00  0.00           C
ATOM   1742  OH  TYR   156     105.263  93.392  67.205  0.00  0.00           O
ATOM   1743  CE2 TYR   156     105.296  91.425  68.555  0.00  0.00           C
ATOM   1744  CD2 TYR   156     105.959  90.281  68.997  0.00  0.00           C
ATOM   1745  H   TYR   156     109.565  88.424  67.145  1.00  0.00           H
ATOM   1746  HA  TYR   156     109.702  89.539  69.829  0.00  0.00           H
ATOM   1747 1HB  TYR   156     107.396  88.358  69.964  0.00  0.00           H
ATOM   1748 2HB  TYR   156     107.629  87.819  68.330  0.00  0.00           H
ATOM   1749  HD1 TYR   156     108.758  90.552  67.084  0.00  0.00           H
ATOM   1750  HE1 TYR   156     107.610  92.568  66.361  0.00  0.00           H
ATOM   1751  HH  TYR   156     104.508  93.523  67.781  0.00  0.00           H
ATOM   1752  HE2 TYR   156     104.337  91.683  68.977  0.00  0.00           H
ATOM   1753  HD2 TYR   156     105.486  89.679  69.760  0.00  0.00           H
ATOM   1754  N   LEU   157     109.860  86.143  69.853  1.00  0.00           N
ATOM   1755  CA  LEU   157     110.345  85.012  70.711  1.00  0.00           C
ATOM   1756  C   LEU   157     111.873  84.971  71.073  1.00  0.00           C
ATOM   1757  O   LEU   157     112.208  84.574  72.191  1.00  0.00           O
ATOM   1758  CB  LEU   157     109.771  83.662  70.181  1.00  0.00           C
ATOM   1759  CG  LEU   157     110.541  82.934  69.039  1.00  0.00           C
ATOM   1760  CD1 LEU   157     111.558  81.907  69.572  1.00  0.00           C
ATOM   1761  CD2 LEU   157     109.575  82.206  68.098  1.00  0.00           C
ATOM   1762  H   LEU   157     109.582  86.019  68.870  1.00  0.00           H
ATOM   1763  HA  LEU   157     109.856  85.147  71.693  1.00  0.00           H
ATOM   1764 1HB  LEU   157     109.664  82.968  71.037  1.00  0.00           H
ATOM   1765 2HB  LEU   157     108.718  83.834  69.881  1.00  0.00           H
ATOM   1766  HG  LEU   157     111.088  83.689  68.443  1.00  0.00           H
ATOM   1767 2HD1 LEU   157     112.317  82.369  70.227  1.00  0.00           H
ATOM   1768 3HD1 LEU   157     111.074  81.105  70.159  1.00  0.00           H
ATOM   1769 1HD1 LEU   157     112.116  81.418  68.750  1.00  0.00           H
ATOM   1770 2HD2 LEU   157     108.993  81.441  68.635  1.00  0.00           H
ATOM   1771 3HD2 LEU   157     108.848  82.902  67.638  1.00  0.00           H
ATOM   1772 1HD2 LEU   157     110.101  81.700  67.267  1.00  0.00           H
ATOM   1773  N   ARG   158     112.794  85.339  70.162  1.00  0.00           N
ATOM   1774  CA  ARG   158     114.267  85.286  70.417  1.00  0.00           C
ATOM   1775  C   ARG   158     114.818  86.178  71.582  1.00  0.00           C
ATOM   1776  O   ARG   158     115.619  85.706  72.392  1.00  0.00           O
ATOM   1777  CB  ARG   158     115.007  85.449  69.057  1.00  0.00           C
ATOM   1778  CG  ARG   158     115.175  86.874  68.458  1.00  0.00           C
ATOM   1779  CD  ARG   158     116.540  87.524  68.779  1.00  0.00           C
ATOM   1780  NE  ARG   158     116.446  89.000  68.662  1.00  0.00           N
ATOM   1781  CZ  ARG   158     117.045  89.775  67.769  1.00  0.00           C
ATOM   1782  NH1 ARG   158     117.835  89.356  66.828  1.00  0.00           N
ATOM   1783  NH2 ARG   158     116.819  91.036  67.853  1.00  0.00           N
ATOM   1784  HE  ARG   158     115.849  89.477  69.353  1.00  0.00           H
ATOM   1785  H   ARG   158     112.401  85.649  69.259  1.00  0.00           H
ATOM   1786  HA  ARG   158     114.482  84.249  70.742  1.00  0.00           H
ATOM   1787 1HB  ARG   158     115.999  84.986  69.177  1.00  0.00           H
ATOM   1788 2HB  ARG   158     114.521  84.802  68.299  1.00  0.00           H
ATOM   1789 1HG  ARG   158     115.054  86.841  67.357  1.00  0.00           H
ATOM   1790 2HG  ARG   158     114.337  87.520  68.789  1.00  0.00           H
ATOM   1791 1HD  ARG   158     116.836  87.294  69.821  1.00  0.00           H
ATOM   1792 2HD  ARG   158     117.337  87.084  68.149  1.00  0.00           H
ATOM   1793 2HH1 ARG   158     117.958  88.343  66.791  1.00  0.00           H
ATOM   1794 1HH1 ARG   158     118.205  90.060  66.191  1.00  0.00           H
ATOM   1795 1HH2 ARG   158     116.085  91.238  68.536  1.00  0.00           H
ATOM   1796 2HH2 ARG   158     117.170  91.627  67.101  1.00  0.00           H
ATOM   1797  N   GLN   159     114.342  87.426  71.705  0.00  0.00           N
ATOM   1798  CA  GLN   159     114.561  88.275  72.911  0.00  0.00           C
ATOM   1799  C   GLN   159     113.899  87.764  74.246  0.00  0.00           C
ATOM   1800  O   GLN   159     114.458  87.994  75.318  0.00  0.00           O
ATOM   1801  CB  GLN   159     114.096  89.718  72.581  0.00  0.00           C
ATOM   1802  CG  GLN   159     114.776  90.433  71.381  0.00  0.00           C
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ATOM	1803	CD	GLN	159	114.427	91.912	71.236	0.00	0.00	C
ATOM	1804	OE1	GLN	159	113.474	92.320	70.582	0.00	0.00	O
ATOM	1805	NE2	GLN	159	115.171	92.782	71.861	0.00	0.00	N
ATOM	1806	H	GLN	159	113.734	87.719	70.929	0.00	0.00	H
ATOM	1807	HA	GLN	159	115.650	88.322	73.109	0.00	0.00	H
ATOM	1808	1HB	GLN	159	114.249	90.337	73.487	0.00	0.00	H
ATOM	1809	2HB	GLN	159	113.003	89.711	72.411	0.00	0.00	H
ATOM	1810	1HG	GLN	159	114.475	89.939	70.438	0.00	0.00	H
ATOM	1811	2HG	GLN	159	115.875	90.305	71.420	0.00	0.00	H
ATOM	1812	1HE2	GLN	159	115.731	92.400	72.632	0.00	0.00	H
ATOM	1813	2HE2	GLN	159	114.805	93.732	71.792	0.00	0.00	H
ATOM	1814	N	ILE	160	112.749	87.059	74.203	0.00	0.00	N
ATOM	1815	CA	ILE	160	112.178	86.320	75.382	0.00	0.00	C
ATOM	1816	C	ILE	160	113.065	85.090	75.820	0.00	0.00	C
ATOM	1817	O	ILE	160	113.349	84.959	77.011	0.00	0.00	O
ATOM	1818	CB	ILE	160	110.665	85.933	75.161	0.00	0.00	C
ATOM	1819	CG2	ILE	160	110.033	85.314	76.441	0.00	0.00	C
ATOM	1820	CG1	ILE	160	109.741	87.100	74.696	0.00	0.00	C
ATOM	1821	CD1	ILE	160	108.408	86.662	74.063	0.00	0.00	C
ATOM	1822	H	ILE	160	112.391	86.927	73.248	0.00	0.00	H
ATOM	1823	HA	ILE	160	112.195	87.020	76.242	0.00	0.00	H
ATOM	1824	HB	ILE	160	110.651	85.163	74.364	0.00	0.00	H
ATOM	1825	1HG2	ILE	160	108.989	84.988	76.278	0.00	0.00	H
ATOM	1826	2HG2	ILE	160	110.580	84.418	76.788	0.00	0.00	H
ATOM	1827	3HG2	ILE	160	110.020	86.029	77.284	0.00	0.00	H
ATOM	1828	1HG1	ILE	160	110.259	87.714	73.936	0.00	0.00	H
ATOM	1829	2HG1	ILE	160	109.554	87.808	75.526	0.00	0.00	H
ATOM	1830	1HD1	ILE	160	107.902	87.513	73.570	0.00	0.00	H
ATOM	1831	2HD1	ILE	160	108.545	85.892	73.285	0.00	0.00	H
ATOM	1832	3HD1	ILE	160	107.708	86.253	74.812	0.00	0.00	H
ATOM	1833	N	VAL	161	113.521	84.213	74.899	0.00	0.00	N
ATOM	1834	CA	VAL	161	114.529	83.137	75.205	0.00	0.00	C
ATOM	1835	C	VAL	161	115.907	83.685	75.750	0.00	0.00	C
ATOM	1836	O	VAL	161	116.400	83.167	76.752	0.00	0.00	O
ATOM	1837	CB	VAL	161	114.681	82.153	73.984	0.00	0.00	C
ATOM	1838	CG1	VAL	161	115.681	80.993	74.226	0.00	0.00	C
ATOM	1839	CG2	VAL	161	113.363	81.472	73.541	0.00	0.00	C
ATOM	1840	H	VAL	161	113.202	84.416	73.940	0.00	0.00	H
ATOM	1841	HA	VAL	161	114.115	82.533	76.037	0.00	0.00	H
ATOM	1842	HB	VAL	161	115.060	82.747	73.126	0.00	0.00	H
ATOM	1843	1HG1	VAL	161	115.804	80.350	73.333	0.00	0.00	H
ATOM	1844	2HG1	VAL	161	116.693	81.358	74.477	0.00	0.00	H
ATOM	1845	3HG1	VAL	161	115.368	80.335	75.059	0.00	0.00	H
ATOM	1846	1HG2	VAL	161	113.504	80.827	72.653	0.00	0.00	H
ATOM	1847	2HG2	VAL	161	112.928	80.840	74.338	0.00	0.00	H
ATOM	1848	3HG2	VAL	161	112.588	82.210	73.260	0.00	0.00	H
ATOM	1849	N	LEU	162	116.504	84.730	75.145	0.00	0.00	N
ATOM	1850	CA	LEU	162	117.649	85.484	75.753	0.00	0.00	C
ATOM	1851	C	LEU	162	117.378	86.204	77.127	0.00	0.00	C
ATOM	1852	O	LEU	162	118.260	86.217	77.988	0.00	0.00	O
ATOM	1853	CB	LEU	162	118.193	86.481	74.690	0.00	0.00	C
ATOM	1854	CG	LEU	162	118.906	85.886	73.448	0.00	0.00	C
ATOM	1855	CD1	LEU	162	119.135	86.980	72.393	0.00	0.00	C
ATOM	1856	CD2	LEU	162	120.255	85.243	73.811	0.00	0.00	C
ATOM	1857	H	LEU	162	116.028	85.052	74.289	0.00	0.00	H
ATOM	1858	HA	LEU	162	118.451	84.756	75.972	0.00	0.00	H
ATOM	1859	1HB	LEU	162	118.894	87.188	75.175	0.00	0.00	H
ATOM	1860	2HB	LEU	162	117.350	87.120	74.357	0.00	0.00	H
ATOM	1861	HG	LEU	162	118.252	85.114	72.991	0.00	0.00	H
ATOM	1862	1HD1	LEU	162	119.596	86.571	71.476	0.00	0.00	H
ATOM	1863	2HD1	LEU	162	118.185	87.452	72.080	0.00	0.00	H
ATOM	1864	3HD1	LEU	162	119.301	87.705	72.757	0.00	0.00	H

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ATOM   1876  CA  CYS   164     114.876  83.737  80.335  1.00  0.00           C
ATOM   1877  C   CYS   164     116.266  83.039  80.567  1.00  0.00           C
ATOM   1878  O   CYS   164     116.521  82.564  81.673  1.00  0.00           O
ATOM   1879  CB  CYS   164     113.829  82.778  79.729  1.00  0.00           C
ATOM   1880  SG  CYS   164     112.154  83.509  79.786  1.00  0.00           S
ATOM   1881  H   CYS   164     114.400  84.992  78.570  1.00  0.00           H
ATOM   1882  HA  CYS   164     114.518  84.010  81.346  1.00  0.00           H
ATOM   1883 1HB  CYS   164     114.081  82.520  78.681  1.00  0.00           H
ATOM   1884 2HB  CYS   164     113.813  81.822  80.285  1.00  0.00           H
ATOM   1885  HG  CYS   164     112.078  83.650  81.109  1.00  0.00           H
ATOM   1886  N   GLN   165     117.185  83.026  79.584  1.00  0.00           N
ATOM   1887  CA  GLN   165     118.630  82.717  79.812  1.00  0.00           C
ATOM   1888  C   GLN   165     119.377  83.597  80.884  1.00  0.00           C
ATOM   1889  O   GLN   165     120.137  83.048  81.686  1.00  0.00           O
ATOM   1890  CB  GLN   165     119.305  82.732  78.409  1.00  0.00           C
ATOM   1891  CG  GLN   165     120.812  82.361  78.337  1.00  0.00           C
ATOM   1892  CD  GLN   165     121.171  80.925  78.714  1.00  0.00           C
ATOM   1893  OE1 GLN   165     121.176  80.021  77.889  1.00  0.00           O
ATOM   1894  NE2 GLN   165     121.483  80.662  79.958  1.00  0.00           N
ATOM   1895  H   GLN   165     116.831  83.380  78.683  1.00  0.00           H
ATOM   1896  HA  GLN   165     118.685  81.679  80.192  1.00  0.00           H
ATOM   1897 1HB  GLN   165     118.748  82.064  77.721  1.00  0.00           H
ATOM   1898 2HB  GLN   165     119.186  83.742  77.971  1.00  0.00           H
ATOM   1899 1HG  GLN   165     121.163  82.514  77.300  1.00  0.00           H
ATOM   1900 2HG  GLN   165     121.416  83.072  78.933  1.00  0.00           H
ATOM   1901 1HE2 GLN   165     121.348  81.425  80.632  1.00  0.00           H
ATOM   1902 2HE2 GLN   165     121.686  79.679  80.146  1.00  0.00           H
ATOM   1903  N   TYR   166     119.158  84.923  80.915  0.00  0.00           N
ATOM   1904  CA  TYR   166     119.568  85.789  82.059  0.00  0.00           C
ATOM   1905  C   TYR   166     118.771  85.539  83.393  0.00  0.00           C
ATOM   1906  O   TYR   166     119.399  85.300  84.425  0.00  0.00           O
ATOM   1907  CB  TYR   166     119.502  87.256  81.545  0.00  0.00           C
ATOM   1908  CG  TYR   166     120.132  88.308  82.473  0.00  0.00           C
ATOM   1909  CD1 TYR   166     121.487  88.633  82.352  0.00  0.00           C
ATOM   1910  CE1 TYR   166     122.045  89.626  83.155  0.00  0.00           C
ATOM   1911  CZ  TYR   166     121.259  90.279  84.099  0.00  0.00           C
ATOM   1912  OH  TYR   166     121.795  91.289  84.845  0.00  0.00           O
ATOM   1913  CE2 TYR   166     119.916  89.950  84.239  0.00  0.00           C
ATOM   1914  CD2 TYR   166     119.349  88.973  83.422  0.00  0.00           C
ATOM   1915  H   TYR   166     118.685  85.361  80.112  1.00  0.00           H
ATOM   1916  HA  TYR   166     120.631  85.572  82.293  0.00  0.00           H
ATOM   1917 1HB  TYR   166     118.451  87.533  81.332  0.00  0.00           H
ATOM   1918 2HB  TYR   166     119.994  87.330  80.555  0.00  0.00           H
ATOM   1919  HD1 TYR   166     122.106  88.133  81.622  0.00  0.00           H
ATOM   1920  HE1 TYR   166     123.087  89.891  83.046  0.00  0.00           H
ATOM   1921  HH  TYR   166     122.244  91.892  84.240  0.00  0.00           H
ATOM   1922  HE2 TYR   166     119.310  90.457  84.974  0.00  0.00           H
ATOM   1923  HD2 TYR   166     118.302  88.727  83.543  0.00  0.00           H
ATOM   1924  N   LEU   167     117.424  85.573  83.383  0.00  0.00           N
ATOM   1925  CA  LEU   167     116.580  85.358  84.599  0.00  0.00           C
ATOM   1926  C   LEU   167     116.762  83.982  85.326  0.00  0.00           C
ATOM   1927  O   LEU   167     116.969  83.963  86.540  0.00  0.00           O
ATOM   1928  CB  LEU   167     115.083  85.622  84.256  0.00  0.00           C
ATOM   1929  CG  LEU   167     114.679  87.034  83.757  0.00  0.00           C
ATOM   1930  CD1 LEU   167     113.194  87.063  83.364  0.00  0.00           C
ATOM   1931  CD2 LEU   167     114.939  88.119  84.808  0.00  0.00           C
ATOM   1932  H   LEU   167     117.014  85.798  82.466  0.00  0.00           H
ATOM   1933  HA  LEU   167     116.884  86.113  85.350  0.00  0.00           H
ATOM   1934 1HB  LEU   167     114.473  85.389  85.151  0.00  0.00           H
ATOM   1935 2HB  LEU   167     114.764  84.870  83.510  0.00  0.00           H
ATOM   1936  HG  LEU   167     115.274  87.289  82.858  0.00  0.00           H
ATOM   1937 1HD1 LEU   167     112.894  88.053  82.971  0.00  0.00           H
ATOM   1938 2HD1 LEU   167     112.964  86.327  82.572  0.00  0.00           H
ATOM   1939 3HD1 LEU   167     112.532  86.847  84.222  0.00  0.00           H
ATOM   1940 1HD2 LEU   167     114.642  89.118  84.443  0.00  0.00           H
ATOM   1941 2HD2 LEU   167     114.388  87.929  85.748  0.00  0.00           H
ATOM   1942 3HD2 LEU   167     116.011  88.196  85.072  0.00  0.00           H
ATOM   1943  N   HIS   168     116.757  82.845  84.609  0.00  0.00           N
ATOM   1944  CA  HIS   168     117.105  81.512  85.190  0.00  0.00           C
ATOM   1945  C   HIS   168     118.576  81.396  85.749  0.00  0.00           C
ATOM   1946  O   HIS   168     118.773  80.818  86.819  0.00  0.00           O
ATOM   1947  CB  HIS   168     116.788  80.395  84.153  0.00  0.00           C
ATOM   1948  CG  HIS   168     115.353  80.235  83.617  0.00  0.00           C
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ATOM	1949	ND1	HIS	168	114.199	80.809	84.143	0.00	0.00	N
ATOM	1950	CE1	HIS	168	113.278	80.323	83.255	0.00	0.00	C
ATOM	1951	NE2	HIS	168	113.675	79.497	82.239	0.00	0.00	N
ATOM	1952	CD2	HIS	168	115.034	79.451	82.498	0.00	0.00	C
ATOM	1953	H	HIS	168	116.578	82.972	83.603	0.00	0.00	H
ATOM	1954	HA	HIS	168	116.440	81.343	86.062	0.00	0.00	H
ATOM	1955	1HB	HIS	168	117.074	79.422	84.594	0.00	0.00	H
ATOM	1956	2HB	HIS	168	117.467	80.521	83.289	0.00	0.00	H
ATOM	1957	HE1	HIS	168	112.235	80.561	83.392	0.00	0.00	H
ATOM	1958	HE2	HIS	168	113.102	78.947	81.590	0.00	0.00	H
ATOM	1959	HD2	HIS	168	115.756	78.876	81.940	0.00	0.00	H
ATOM	1960	N	ARG	169	119.587	81.991	85.080	1.00	0.00	N
ATOM	1961	CA	ARG	169	120.937	82.244	85.682	1.00	0.00	C
ATOM	1962	C	ARG	169	120.977	83.160	86.968	1.00	0.00	C
ATOM	1963	O	ARG	169	121.743	82.871	87.888	1.00	0.00	O
ATOM	1964	CB	ARG	169	121.828	82.766	84.521	1.00	0.00	C
ATOM	1965	CG	ARG	169	123.343	82.852	84.825	1.00	0.00	C
ATOM	1966	CD	ARG	169	124.142	83.372	83.619	1.00	0.00	C
ATOM	1967	NE	ARG	169	125.581	83.393	83.981	1.00	0.00	N
ATOM	1968	CZ	ARG	169	126.573	83.759	83.183	1.00	0.00	C
ATOM	1969	NH1	ARG	169	126.421	84.150	81.954	1.00	0.00	N
ATOM	1970	NH2	ARG	169	127.763	83.721	83.667	1.00	0.00	N
ATOM	1971	HE	ARG	169	125.830	83.099	84.936	1.00	0.00	H
ATOM	1972	H	ARG	169	119.258	82.535	84.276	1.00	0.00	H
ATOM	1973	HA	ARG	169	121.348	81.266	86.002	1.00	0.00	H
ATOM	1974	1HB	ARG	169	121.700	82.114	83.635	1.00	0.00	H
ATOM	1975	2HB	ARG	169	121.462	83.761	84.197	1.00	0.00	H
ATOM	1976	1HG	ARG	169	123.525	83.511	85.698	1.00	0.00	H
ATOM	1977	2HG	ARG	169	123.729	81.859	85.131	1.00	0.00	H
ATOM	1978	1HD	ARG	169	123.973	82.723	82.737	1.00	0.00	H
ATOM	1979	2HD	ARG	169	123.797	84.390	83.344	1.00	0.00	H
ATOM	1980	2HH1	ARG	169	125.445	84.158	81.655	1.00	0.00	H
ATOM	1981	1HH1	ARG	169	127.263	84.410	81.442	1.00	0.00	H
ATOM	1982	1HH2	ARG	169	127.763	83.411	84.641	1.00	0.00	H
ATOM	1983	2HH2	ARG	169	128.535	84.007	83.067	1.00	0.00	H
ATOM	1984	N	ASN	170	120.138	84.208	87.078	1.00	0.00	N
ATOM	1985	CA	ASN	170	119.868	84.914	88.374	1.00	0.00	C
ATOM	1986	C	ASN	170	119.114	84.109	89.511	1.00	0.00	C
ATOM	1987	O	ASN	170	118.897	84.666	90.590	1.00	0.00	O
ATOM	1988	CB	ASN	170	119.043	86.208	88.075	1.00	0.00	C
ATOM	1989	CG	ASN	170	119.476	87.253	87.043	1.00	0.00	C
ATOM	1990	OD1	ASN	170	118.647	87.828	86.350	1.00	0.00	O
ATOM	1991	ND2	ASN	170	120.734	87.585	86.923	1.00	0.00	N
ATOM	1992	H	ASN	170	119.600	84.408	86.222	1.00	0.00	H
ATOM	1993	HA	ASN	170	120.836	85.216	88.819	1.00	0.00	H
ATOM	1994	1HB	ASN	170	118.016	85.911	87.792	1.00	0.00	H
ATOM	1995	2HB	ASN	170	118.903	86.769	89.016	1.00	0.00	H
ATOM	1996	1HD2	ASN	170	120.898	88.227	86.142	1.00	0.00	H
ATOM	1997	2HD2	ASN	170	121.406	86.966	87.382	1.00	0.00	H
ATOM	1998	N	ARG	171	118.659	82.858	89.280	1.00	0.00	N
ATOM	1999	CA	ARG	171	117.640	82.151	90.127	1.00	0.00	C
ATOM	2000	C	ARG	171	116.210	82.824	90.209	1.00	0.00	C
ATOM	2001	O	ARG	171	115.514	82.730	91.223	1.00	0.00	O
ATOM	2002	CB	ARG	171	118.236	81.706	91.497	1.00	0.00	C
ATOM	2003	CG	ARG	171	119.399	80.683	91.421	1.00	0.00	C
ATOM	2004	CD	ARG	171	119.917	80.277	92.807	1.00	0.00	C
ATOM	2005	NE	ARG	171	120.996	79.272	92.633	1.00	0.00	N
ATOM	2006	CZ	ARG	171	121.728	78.749	93.607	1.00	0.00	C
ATOM	2007	NH1	ARG	171	121.590	79.037	94.866	1.00	0.00	N
ATOM	2008	NH2	ARG	171	122.652	77.900	93.271	1.00	0.00	N
ATOM	2009	HE	ARG	171	121.194	78.955	91.671	1.00	0.00	H
ATOM	2010	H	ARG	171	119.508	82.485	88.371	1.00	0.00	H

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ATOM   2022  N   VAL  172     115.741  83.442  89.110  1.00  0.00           N
ATOM   2023  CA  VAL  172     114.438  84.169  89.046  1.00  0.00           C
ATOM   2024  C   VAL  172     113.496  83.370  88.083  1.00  0.00           C
ATOM   2025  O   VAL  172     113.552  83.505  86.855  1.00  0.00           O
ATOM   2026  CB  VAL  172     114.661  85.671  88.631  1.00  0.00           C
ATOM   2027  CG1 VAL  172     113.351  86.468  88.415  1.00  0.00           C
ATOM   2028  CG2 VAL  172     115.491  86.480  89.657  1.00  0.00           C
ATOM   2029  H   VAL  172     116.426  83.513  88.344  1.00  0.00           H
ATOM   2030  HA  VAL  172     113.959  84.202  90.047  1.00  0.00           H
ATOM   2031  HB  VAL  172     115.214  85.677  87.669  1.00  0.00           H
ATOM   2032 1HG1 VAL  172     112.732  86.513  89.332  1.00  0.00           H
ATOM   2033 2HG1 VAL  172     113.547  87.510  88.101  1.00  0.00           H
ATOM   2034 3HG1 VAL  172     112.721  86.025  87.621  1.00  0.00           H
ATOM   2035 2HG2 VAL  172     116.478  86.016  89.846  1.00  0.00           H
ATOM   2036 3HG2 VAL  172     115.697  87.510  89.309  1.00  0.00           H
ATOM   2037 1HG2 VAL  172     114.986  86.556  90.638  1.00  0.00           H
ATOM   2038  N   ILE  173     112.575  82.575  88.653  0.00  0.00           N
ATOM   2039  CA  ILE  173     111.447  81.954  87.886  0.00  0.00           C
ATOM   2040  C   ILE  173     110.383  83.074  87.611  0.00  0.00           C
ATOM   2041  O   ILE  173     109.709  83.512  88.544  0.00  0.00           O
ATOM   2042  CB  ILE  173     110.844  80.716  88.658  0.00  0.00           C
ATOM   2043  CG2 ILE  173     109.635  80.078  87.912  0.00  0.00           C
ATOM   2044  CG1 ILE  173     111.881  79.595  88.975  0.00  0.00           C
ATOM   2045  CD1 ILE  173     111.442  78.565  90.033  0.00  0.00           C
ATOM   2046  H   ILE  173     112.632  82.538  89.675  0.00  0.00           H
ATOM   2047  HA  ILE  173     111.836  81.577  86.918  0.00  0.00           H
ATOM   2048  HB  ILE  173     110.467  81.102  89.627  0.00  0.00           H
ATOM   2049 1HG2 ILE  173     109.151  79.289  88.517  0.00  0.00           H
ATOM   2050 2HG2 ILE  173     108.838  80.813  87.695  0.00  0.00           H
ATOM   2051 3HG2 ILE  173     109.929  79.606  86.958  0.00  0.00           H
ATOM   2052 1HG1 ILE  173     112.824  80.045  89.341  0.00  0.00           H
ATOM   2053 2HG1 ILE  173     112.172  79.077  88.044  0.00  0.00           H
ATOM   2054 1HD1 ILE  173     112.255  77.853  90.265  0.00  0.00           H
ATOM   2055 2HD1 ILE  173     111.160  79.050  90.988  0.00  0.00           H
ATOM   2056 3HD1 ILE  173     110.575  77.962  89.706  0.00  0.00           H
ATOM   2057  N   HIS  174     110.237  83.550  86.361  1.00  0.00           N
ATOM   2058  CA  HIS  174     109.317  84.693  86.059  1.00  0.00           C
ATOM   2059  C   HIS  174     107.793  84.449  86.376  1.00  0.00           C
ATOM   2060  O   HIS  174     107.197  85.215  87.138  1.00  0.00           O
ATOM   2061  CB  HIS  174     109.621  85.167  84.608  1.00  0.00           C
ATOM   2062  CG  HIS  174     108.991  86.510  84.245  1.00  0.00           C
ATOM   2063  ND1 HIS  174     109.547  87.720  84.610  1.00  0.00           N
ATOM   2064  CE1 HIS  174     108.528  88.561  84.240  1.00  0.00           C
ATOM   2065  NE2 HIS  174     107.408  88.047  83.646  1.00  0.00           N
ATOM   2066  CD2 HIS  174     107.722  86.700  83.677  1.00  0.00           C
ATOM   2067  H   HIS  174     111.089  83.401  85.808  1.00  0.00           H
ATOM   2068  HA  HIS  174     109.616  85.530  86.728  1.00  0.00           H
ATOM   2069 1HB  HIS  174     110.714  85.272  84.465  1.00  0.00           H
ATOM   2070 2HB  HIS  174     109.312  84.405  83.873  1.00  0.00           H
ATOM   2071  HE1 HIS  174     108.594  89.618  84.467  1.00  0.00           H
ATOM   2072  HE2 HIS  174     106.492  88.497  83.525  1.00  0.00           H
ATOM   2073  HD2 HIS  174     107.043  85.901  83.421  1.00  0.00           H
ATOM   2074  N   ARG  175     107.160  83.405  85.801  0.00  0.00           N
ATOM   2075  CA  ARG  175     105.738  83.015  86.076  0.00  0.00           C
ATOM   2076  C   ARG  175     104.626  83.935  85.455  0.00  0.00           C
ATOM   2077  O   ARG  175     103.710  83.427  84.802  0.00  0.00           O
ATOM   2078  CB  ARG  175     105.530  82.631  87.571  0.00  0.00           C
ATOM   2079  CG  ARG  175     104.378  81.637  87.838  0.00  0.00           C
ATOM   2080  CD  ARG  175     104.296  81.222  89.315  0.00  0.00           C
ATOM   2081  NE  ARG  175     103.290  80.140  89.415  0.00  0.00           N
ATOM   2082  CZ  ARG  175     102.838  79.593  90.531  0.00  0.00           C
ATOM   2083  NH1 ARG  175     103.214  79.931  91.729  0.00  0.00           N
ATOM   2084  NH2 ARG  175     101.966  78.668  90.400  0.00  0.00           N
ATOM   2085  HE  ARG  175     102.905  79.778  88.530  1.00  0.00           H
ATOM   2086  H   ARG  175     107.738  82.919  85.104  0.00  0.00           H
ATOM   2087  HA  ARG  175     105.622  82.068  85.513  0.00  0.00           H
ATOM   2088 1HB  ARG  175     105.397  83.551  88.171  0.00  0.00           H
ATOM   2089 2HB  ARG  175     106.465  82.177  87.958  0.00  0.00           H
ATOM   2090 1HG  ARG  175     104.517  80.733  87.210  0.00  0.00           H
ATOM   2091 2HG  ARG  175     103.406  82.064  87.515  0.00  0.00           H
ATOM   2092 1HD  ARG  175     104.009  82.089  89.943  0.00  0.00           H
ATOM   2093 2HD  ARG  175     105.280  80.863  89.681  0.00  0.00           H
ATOM   2094 1HH1 ARG  175     102.744  79.451  92.498  0.00  0.00           H
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ATOM	2095	2HH1	ARG	175	103.889	80.695	91.751	0.00	0.00	H
ATOM	2096	1HH2	ARG	175	101.643	78.167	91.237	0.00	0.00	H
ATOM	2097	2HH2	ARG	175	101.804	78.446	89.417	0.00	0.00	H
ATOM	2098	N	ASP	176	104.702	85.268	85.615	0.00	0.00	N
ATOM	2099	CA	ASP	176	103.764	86.234	84.968	0.00	0.00	C
ATOM	2100	C	ASP	176	104.080	86.497	83.442	0.00	0.00	C
ATOM	2101	O	ASP	176	104.454	87.605	83.049	0.00	0.00	O
ATOM	2102	CB	ASP	176	103.818	87.483	85.894	0.00	0.00	C
ATOM	2103	CG	ASP	176	102.699	88.484	85.653	0.00	0.00	C
ATOM	2104	OD1	ASP	176	101.504	88.205	85.698	0.00	0.00	O
ATOM	2105	OD2	ASP	176	103.054	89.672	85.637	0.00	0.00	O
ATOM	2106	H	ASP	176	105.525	85.562	86.163	0.00	0.00	H
ATOM	2107	HA	ASP	176	102.735	85.823	85.015	0.00	0.00	H
ATOM	2108	1HB	ASP	176	104.797	87.993	85.798	0.00	0.00	H
ATOM	2109	2HB	ASP	176	103.748	87.209	86.962	0.00	0.00	H
ATOM	2110	N	LEU	177	103.924	85.481	82.572	0.00	0.00	N
ATOM	2111	CA	LEU	177	104.341	85.556	81.137	0.00	0.00	C
ATOM	2112	C	LEU	177	103.112	85.411	80.177	0.00	0.00	C
ATOM	2113	O	LEU	177	102.648	84.308	79.872	0.00	0.00	O
ATOM	2114	CB	LEU	177	105.476	84.511	80.915	0.00	0.00	C
ATOM	2115	CG	LEU	177	106.235	84.562	79.560	0.00	0.00	C
ATOM	2116	CD1	LEU	177	106.906	85.921	79.284	0.00	0.00	C
ATOM	2117	CD2	LEU	177	107.333	83.485	79.529	0.00	0.00	C
ATOM	2118	H	LEU	177	103.702	84.587	83.030	0.00	0.00	H
ATOM	2119	HA	LEU	177	104.805	86.542	80.937	0.00	0.00	H
ATOM	2120	1HB	LEU	177	105.054	83.496	81.051	0.00	0.00	H
ATOM	2121	2HB	LEU	177	106.224	84.609	81.725	0.00	0.00	H
ATOM	2122	HG	LEU	177	105.517	84.348	78.741	0.00	0.00	H
ATOM	2123	1HD1	LEU	177	107.505	85.902	78.353	0.00	0.00	H
ATOM	2124	2HD1	LEU	177	106.167	86.732	79.150	0.00	0.00	H
ATOM	2125	3HD1	LEU	177	107.586	86.228	80.101	0.00	0.00	H
ATOM	2126	1HD2	LEU	177	107.855	83.463	78.556	0.00	0.00	H
ATOM	2127	2HD2	LEU	177	108.102	83.646	80.307	0.00	0.00	H
ATOM	2128	3HD2	LEU	177	106.926	82.471	79.685	0.00	0.00	H
ATOM	2129	N	LYS	178	102.583	86.554	79.709	0.00	0.00	N
ATOM	2130	CA	LYS	178	101.463	86.610	78.722	0.00	0.00	C
ATOM	2131	C	LYS	178	101.689	87.771	77.676	0.00	0.00	C
ATOM	2132	O	LYS	178	102.744	88.413	77.632	0.00	0.00	O
ATOM	2133	CB	LYS	178	100.114	86.647	79.527	0.00	0.00	C
ATOM	2134	CG	LYS	178	99.771	88.005	80.244	0.00	0.00	C
ATOM	2135	CD	LYS	178	98.457	88.773	79.928	0.00	0.00	C
ATOM	2136	CE	LYS	178	98.363	90.078	80.774	0.00	0.00	C
ATOM	2137	NZ	LYS	178	97.371	91.082	80.284	0.00	0.00	N
ATOM	2138	1HZ	LYS	178	96.334	90.864	80.118	1.00	0.00	H
ATOM	2139	2HZ	LYS	178	97.357	92.061	80.681	1.00	0.00	H
ATOM	2140	3HZ	LYS	178	97.360	91.463	79.301	1.00	0.00	H
ATOM	2141	H	LYS	178	103.132	87.388	79.934	0.00	0.00	H
ATOM	2142	HA	LYS	178	101.469	85.678	78.119	0.00	0.00	H
ATOM	2143	1HB	LYS	178	100.182	85.941	80.379	0.00	0.00	H
ATOM	2144	2HB	LYS	178	99.318	86.209	78.895	0.00	0.00	H
ATOM	2145	1HG	LYS	178	100.614	88.710	80.085	0.00	0.00	H
ATOM	2146	2HG	LYS	178	99.828	87.850	81.343	0.00	0.00	H
ATOM	2147	1HD	LYS	178	97.563	88.150	80.119	0.00	0.00	H
ATOM	2148	2HD	LYS	178	98.407	89.015	78.850	0.00	0.00	H
ATOM	2149	1HE	LYS	178	99.353	90.577	80.849	0.00	0.00	H
ATOM	2150	2HE	LYS	178	98.140	89.833	81.834	0.00	0.00	H
ATOM	2151	N	LEU	179	100.665	88.092	76.867	1.00	0.00	N
ATOM	2152	CA	LEU	179	100.661	89.288	75.979	1.00	0.00	C
ATOM	2153	C	LEU	179	100.758	90.666	76.713	1.00	0.00	C
ATOM	2154	O	LEU	179	101.659	91.433	76.379	1.00	0.00	O
ATOM	2155	CD	LEU	179	99.451	89.238	75.007	1.00	0.00	C
ATOM	2156	[illegible]	[illegible]	179	99.[illegible]	90.[illegible]	75.[illegible]	1.00	0.00	[illegible]

ATOM	2168	3HD2	LEU	179	98.936	89.497	72.259	1.00	0.00	H
ATOM	2169	1HD2	LEU	179	98.605	87.800	71.899	1.00	0.00	H
ATOM	2170	N	GLY	180	99.916	90.992	77.712	1.00	0.00	N
ATOM	2171	CA	GLY	180	100.099	92.232	78.527	1.00	0.00	C
ATOM	2172	C	GLY	180	101.529	92.588	79.036	1.00	0.00	C
ATOM	2173	O	GLY	180	102.060	93.647	78.710	1.00	0.00	O
ATOM	2174	H	GLY	180	99.039	90.461	77.744	1.00	0.00	H
ATOM	2175	1HA	GLY	180	99.812	93.071	77.875	1.00	0.00	H
ATOM	2176	2HA	GLY	180	99.394	92.319	79.367	1.00	0.00	H
ATOM	2177	N	ASN	181	102.174	91.645	79.727	0.00	0.00	N
ATOM	2178	CA	ASN	181	103.474	91.871	80.434	0.00	0.00	C
ATOM	2179	C	ASN	181	104.829	91.922	79.623	0.00	0.00	C
ATOM	2180	O	ASN	181	105.920	91.917	80.207	0.00	0.00	O
ATOM	2181	CB	ASN	181	103.567	90.754	81.519	0.00	0.00	C
ATOM	2182	CG	ASN	181	102.405	90.641	82.505	0.00	0.00	C
ATOM	2183	OD1	ASN	181	101.450	89.904	82.283	0.00	0.00	O
ATOM	2184	ND2	ASN	181	102.429	91.382	83.570	0.00	0.00	N
ATOM	2185	H	ASN	181	101.561	90.881	80.025	0.00	0.00	H
ATOM	2186	HA	ASN	181	103.420	92.840	80.969	0.00	0.00	H
ATOM	2187	1HB	ASN	181	104.500	90.872	82.106	0.00	0.00	H
ATOM	2188	2HB	ASN	181	103.685	89.766	81.039	0.00	0.00	H
ATOM	2189	1HD2	ASN	181	102.021	90.827	84.338	0.00	0.00	H
ATOM	2190	2HD2	ASN	181	103.337	91.837	83.699	0.00	0.00	H
ATOM	2191	N	LEU	182	104.794	92.001	78.289	0.00	0.00	N
ATOM	2192	CA	LEU	182	106.015	92.163	77.449	0.00	0.00	C
ATOM	2193	C	LEU	182	105.850	93.462	76.595	0.00	0.00	C
ATOM	2194	O	LEU	182	104.848	93.643	75.902	0.00	0.00	O
ATOM	2195	CB	LEU	182	106.188	90.902	76.560	0.00	0.00	C
ATOM	2196	CG	LEU	182	106.477	89.531	77.242	0.00	0.00	C
ATOM	2197	CD1	LEU	182	106.212	88.418	76.223	0.00	0.00	C
ATOM	2198	CD2	LEU	182	107.914	89.431	77.773	0.00	0.00	C
ATOM	2199	H	LEU	182	103.841	92.184	77.945	0.00	0.00	H
ATOM	2200	HA	LEU	182	106.927	92.272	78.072	0.00	0.00	H
ATOM	2201	1HB	LEU	182	106.998	91.117	75.844	0.00	0.00	H
ATOM	2202	2HB	LEU	182	105.275	90.809	75.941	0.00	0.00	H
ATOM	2203	HG	LEU	182	105.775	89.389	78.091	0.00	0.00	H
ATOM	2204	1HD1	LEU	182	106.449	87.416	76.624	0.00	0.00	H
ATOM	2205	2HD1	LEU	182	105.148	88.392	75.917	0.00	0.00	H
ATOM	2206	3HD1	LEU	182	106.808	88.561	75.304	0.00	0.00	H
ATOM	2207	1HD2	LEU	182	108.125	88.438	78.211	0.00	0.00	H
ATOM	2208	2HD2	LEU	182	108.666	89.603	76.980	0.00	0.00	H
ATOM	2209	3HD2	LEU	182	108.102	90.172	78.570	0.00	0.00	H
ATOM	2210	N	PHE	183	106.816	94.384	76.619	1.00	0.00	N
ATOM	2211	CA	PHE	183	106.566	95.801	76.213	1.00	0.00	C
ATOM	2212	C	PHE	183	107.378	96.162	74.934	1.00	0.00	C
ATOM	2213	O	PHE	183	108.602	96.004	74.910	1.00	0.00	O
ATOM	2214	CB	PHE	183	106.879	96.721	77.437	1.00	0.00	C
ATOM	2215	CG	PHE	183	105.873	96.583	78.598	1.00	0.00	C
ATOM	2216	CD1	PHE	183	104.710	97.353	78.601	1.00	0.00	C
ATOM	2217	CE1	PHE	183	103.664	97.046	79.467	1.00	0.00	C
ATOM	2218	CZ	PHE	183	103.797	96.002	80.375	1.00	0.00	C
ATOM	2219	CE2	PHE	183	104.987	95.288	80.441	1.00	0.00	C
ATOM	2220	CD2	PHE	183	106.024	95.575	79.557	1.00	0.00	C
ATOM	2221	H	PHE	183	107.542	94.195	77.325	1.00	0.00	H
ATOM	2222	HA	PHE	183	105.494	95.964	75.974	1.00	0.00	H
ATOM	2223	1HB	PHE	183	107.909	96.554	77.805	1.00	0.00	H
ATOM	2224	2HB	PHE	183	106.890	97.776	77.103	1.00	0.00	H
ATOM	2225	HD1	PHE	183	104.614	98.187	77.924	1.00	0.00	H
ATOM	2226	HE1	PHE	183	102.761	97.638	79.466	1.00	0.00	H
ATOM	2227	HZ	PHE	183	102.988	95.770	81.054	1.00	0.00	H
ATOM	2228	HE2	PHE	183	105.094	94.496	81.163	1.00	0.00	H
ATOM	2229	HD2	PHE	183	106.917	94.968	79.579	1.00	0.00	H
ATOM	2230	N	LEU	184	106.730	96.690	73.873	1.00	0.00	N
ATOM	2231	CA	LEU	184	107.416	97.309	72.691	1.00	0.00	C
ATOM	2232	C	LEU	184	108.064	98.692	73.028	1.00	0.00	C
ATOM	2233	O	LEU	184	107.333	99.660	73.283	1.00	0.00	O
ATOM	2234	CB	LEU	184	106.409	97.532	71.512	1.00	0.00	C
ATOM	2235	CG	LEU	184	106.138	96.389	70.506	1.00	0.00	C
ATOM	2236	CD1	LEU	184	105.052	96.846	69.514	1.00	0.00	C
ATOM	2237	CD2	LEU	184	107.372	96.012	69.667	1.00	0.00	C
ATOM	2238	H	LEU	184	105.739	96.918	74.050	1.00	0.00	H
ATOM	2239	HA	LEU	184	108.217	96.630	72.340	1.00	0.00	H
ATOM	2240	1HB	LEU	184	105.456	97.912	71.919	1.00	0.00	H

ATOM	2241	2HB	LEU	184	106.746	98.394	70.898	1.00	0.00	H
ATOM	2242	HG	LEU	184	105.777	95.497	71.059	1.00	0.00	H
ATOM	2243	2HD1	LEU	184	104.139	97.190	70.031	1.00	0.00	H
ATOM	2244	3HD1	LEU	184	105.390	97.690	68.883	1.00	0.00	H
ATOM	2245	1HD1	LEU	184	104.757	96.030	68.831	1.00	0.00	H
ATOM	2246	2HD2	LEU	184	107.705	95.937	69.013	1.00	0.00	H
ATOM	2247	3HD2	LEU	184	108.239	95.724	70.287	1.00	0.00	H
ATOM	2248	1HD2	LEU	184	107.163	95.145	69.011	1.00	0.00	H
ATOM	2249	N	ASN	185	109.403	98.774	73.058	1.00	0.00	N
ATOM	2250	CA	ASN	185	110.106	100.086	73.132	1.00	0.00	C
ATOM	2251	C	ASN	185	110.042	100.930	71.806	1.00	0.00	C
ATOM	2252	O	ASN	185	109.564	100.485	70.758	1.00	0.00	O
ATOM	2253	CB	ASN	185	111.522	99.846	73.732	1.00	0.00	C
ATOM	2254	CG	ASN	185	112.608	99.236	72.837	1.00	0.00	C
ATOM	2255	OD1	ASN	185	112.593	99.298	71.615	1.00	0.00	O
ATOM	2256	ND2	ASN	185	113.632	98.680	73.422	1.00	0.00	N
ATOM	2257	H	ASN	185	109.889	97.875	72.930	1.00	0.00	H
ATOM	2258	HA	ASN	185	109.576	100.716	73.879	1.00	0.00	H
ATOM	2259	1HB	ASN	185	111.919	100.816	74.083	1.00	0.00	H
ATOM	2260	2HB	ASN	185	111.419	99.249	74.657	1.00	0.00	H
ATOM	2261	1HD2	ASN	185	114.326	98.305	72.770	1.00	0.00	H
ATOM	2262	2HD2	ASN	185	113.566	98.525	74.431	1.00	0.00	H
ATOM	2263	N	GLU	186	110.562	102.162	71.853	1.00	0.00	N
ATOM	2264	CA	GLU	186	110.544	103.106	70.696	1.00	0.00	C
ATOM	2265	C	GLU	186	111.399	102.718	69.427	1.00	0.00	C
ATOM	2266	O	GLU	186	111.099	103.204	68.337	1.00	0.00	O
ATOM	2267	CB	GLU	186	110.887	104.518	71.262	1.00	0.00	C
ATOM	2268	CG	GLU	186	109.836	105.203	72.195	1.00	0.00	C
ATOM	2269	CD	GLU	186	109.642	104.655	73.619	1.00	0.00	C
ATOM	2270	OE1	GLU	186	110.476	103.990	74.228	1.00	0.00	O
ATOM	2271	OE2	GLU	186	108.515	104.880	74.100	1.00	0.00	O
ATOM	2272	H	GLU	186	110.799	102.491	72.797	1.00	0.00	H
ATOM	2273	HA	GLU	186	109.504	103.157	70.315	1.00	0.00	H
ATOM	2274	1HB	GLU	186	111.880	104.501	71.757	1.00	0.00	H
ATOM	2275	2HB	GLU	186	111.034	105.199	70.400	1.00	0.00	H
ATOM	2276	1HG	GLU	186	110.104	106.268	72.311	1.00	0.00	H
ATOM	2277	2HG	GLU	186	108.852	105.215	71.690	1.00	0.00	H
ATOM	2278	N	ASP	187	112.403	101.825	69.536	1.00	0.00	N
ATOM	2279	CA	ASP	187	112.999	101.111	68.358	1.00	0.00	C
ATOM	2280	C	ASP	187	112.360	99.707	67.989	1.00	0.00	C
ATOM	2281	O	ASP	187	112.928	98.972	67.175	1.00	0.00	O
ATOM	2282	CB	ASP	187	114.526	100.991	68.633	1.00	0.00	C
ATOM	2283	CG	ASP	187	115.313	102.299	68.593	1.00	0.00	C
ATOM	2284	OD1	ASP	187	115.655	102.860	67.559	1.00	0.00	O
ATOM	2285	OD2	ASP	187	115.596	102.774	69.835	1.00	0.00	O
ATOM	2286	H	ASP	187	112.486	101.438	70.483	1.00	0.00	H
ATOM	2287	HA	ASP	187	112.875	101.719	67.437	1.00	0.00	H
ATOM	2288	1HB	ASP	187	114.712	100.468	69.590	1.00	0.00	H
ATOM	2289	2HB	ASP	187	114.992	100.341	67.870	1.00	0.00	H
ATOM	2290	N	LEU	188	111.182	99.345	68.536	1.00	0.00	N
ATOM	2291	CA	LEU	188	110.435	98.074	68.258	1.00	0.00	C
ATOM	2292	C	LEU	188	111.031	96.740	68.850	1.00	0.00	C
ATOM	2293	O	LEU	188	110.984	95.685	68.210	1.00	0.00	O
ATOM	2294	CB	LEU	188	109.963	97.964	66.770	1.00	0.00	C
ATOM	2295	CG	LEU	188	109.099	99.113	66.185	1.00	0.00	C
ATOM	2296	CD1	LEU	188	108.906	98.904	64.675	1.00	0.00	C
ATOM	2297	CD2	LEU	188	107.720	99.221	66.860	1.00	0.00	C
ATOM	2298	H	LEU	188	110.807	100.045	69.191	1.00	0.00	H
ATOM	2299	HA	LEU	188	109.504	98.180	68.044	1.00	0.00	H
ATOM	2300	1HB	LEU	188	110.866	97.831	66.144	1.00	0.00	H
ATOM	2301	2HB	LEU	188	109.408	97.011	66.643	1.00	0.00	H
ATOM	2302	HG	LEU	188	108.136	100.172	66.637	1.00	0.00	H

ATOM	2314	CG	GLU	189	114.656	95.681	69.821	1.00	0.00	C
ATOM	2315	CD	GLU	189	114.692	96.837	68.832	1.00	0.00	C
ATOM	2316	OE1	GLU	189	115.281	97.892	69.046	1.00	0.00	O
ATOM	2317	OE2	GLU	189	113.970	96.585	67.707	1.00	0.00	O
ATOM	2318	H	GLU	189	111.640	97.704	70.480	1.00	0.00	H
ATOM	2319	HA	GLU	189	112.131	94.686	70.075	1.00	0.00	H
ATOM	2320	1HB	GLU	189	113.790	96.916	71.405	1.00	0.00	H
ATOM	2321	2HB	GLU	189	114.042	95.267	71.843	1.00	0.00	H
ATOM	2322	1HG	GLU	189	115.685	95.563	70.206	1.00	0.00	H
ATOM	2323	2HG	GLU	189	114.440	94.731	69.294	1.00	0.00	H
ATOM	2324	N	VAL	190	111.664	93.866	72.489	1.00	0.00	N
ATOM	2325	CA	VAL	190	111.100	93.293	73.754	1.00	0.00	C
ATOM	2326	C	VAL	190	111.790	93.877	75.036	1.00	0.00	C
ATOM	2327	O	VAL	190	112.974	93.637	75.298	1.00	0.00	O
ATOM	2328	CB	VAL	190	111.177	91.721	73.750	1.00	0.00	C
ATOM	2329	CG1	VAL	190	110.578	91.047	75.010	1.00	0.00	C
ATOM	2330	CG2	VAL	190	110.495	91.026	72.548	1.00	0.00	C
ATOM	2331	H	VAL	190	112.242	93.298	71.855	1.00	0.00	H
ATOM	2332	HA	VAL	190	110.025	93.542	73.801	1.00	0.00	H
ATOM	2333	HB	VAL	190	112.252	91.463	73.722	1.00	0.00	H
ATOM	2334	1HG1	VAL	190	109.496	91.252	75.118	1.00	0.00	H
ATOM	2335	2HG1	VAL	190	110.706	89.949	74.991	1.00	0.00	H
ATOM	2336	3HG1	VAL	190	111.068	91.390	75.941	1.00	0.00	H
ATOM	2337	2HG2	VAL	190	110.881	91.382	71.576	1.00	0.00	H
ATOM	2338	3HG2	VAL	190	110.658	89.933	72.556	1.00	0.00	H
ATOM	2339	1HG2	VAL	190	109.401	91.178	72.544	1.00	0.00	H
ATOM	2340	N	LYS	191	110.996	94.554	75.872	1.00	0.00	N
ATOM	2341	CA	LYS	191	111.369	94.885	77.269	1.00	0.00	C
ATOM	2342	C	LYS	191	110.423	94.113	78.258	1.00	0.00	C
ATOM	2343	O	LYS	191	109.215	94.364	78.306	1.00	0.00	O
ATOM	2344	CB	LYS	191	111.259	96.423	77.448	1.00	0.00	C
ATOM	2345	CG	LYS	191	112.257	97.343	76.706	1.00	0.00	C
ATOM	2346	CD	LYS	191	113.703	97.231	77.229	1.00	0.00	C
ATOM	2347	CE	LYS	191	114.545	98.495	76.998	1.00	0.00	C
ATOM	2348	NZ	LYS	191	115.860	98.307	77.636	1.00	0.00	N
ATOM	2349	1HZ	LYS	191	116.437	99.148	77.489	1.00	0.00	H
ATOM	2350	2HZ	LYS	191	115.733	98.151	78.646	1.00	0.00	H
ATOM	2351	3HZ	LYS	191	116.331	97.491	77.220	1.00	0.00	H
ATOM	2352	H	LYS	191	110.119	94.893	75.451	1.00	0.00	H
ATOM	2353	HA	LYS	191	112.417	94.601	77.489	1.00	0.00	H
ATOM	2354	1HB	LYS	191	110.229	96.745	77.190	1.00	0.00	H
ATOM	2355	2HB	LYS	191	111.347	96.649	78.525	1.00	0.00	H
ATOM	2356	1HG	LYS	191	112.222	97.146	75.616	1.00	0.00	H
ATOM	2357	2HG	LYS	191	111.899	98.383	76.832	1.00	0.00	H
ATOM	2358	1HD	LYS	191	113.684	97.025	78.314	1.00	0.00	H
ATOM	2359	2HD	LYS	191	114.192	96.343	76.780	1.00	0.00	H
ATOM	2360	1HE	LYS	191	114.675	98.701	75.921	1.00	0.00	H
ATOM	2361	2HE	LYS	191	114.048	99.385	77.436	1.00	0.00	H
ATOM	2362	N	ILE	192	110.954	93.189	79.078	1.00	0.00	N
ATOM	2363	CA	ILE	192	110.156	92.448	80.114	1.00	0.00	C
ATOM	2364	C	ILE	192	109.807	93.417	81.306	1.00	0.00	C
ATOM	2365	O	ILE	192	110.706	93.999	81.924	1.00	0.00	O
ATOM	2366	CB	ILE	192	110.905	91.140	80.577	1.00	0.00	C
ATOM	2367	CG1	ILE	192	111.266	90.151	79.424	1.00	0.00	C
ATOM	2368	CG2	ILE	192	110.090	90.351	81.640	1.00	0.00	C
ATOM	2369	CD1	ILE	192	112.362	89.124	79.760	1.00	0.00	C
ATOM	2370	H	ILE	192	111.953	92.986	78.923	1.00	0.00	H
ATOM	2371	HA	ILE	192	109.209	92.115	79.643	1.00	0.00	H
ATOM	2372	HB	ILE	192	111.853	91.469	81.050	1.00	0.00	H
ATOM	2373	1HG1	ILE	192	110.364	89.623	79.069	1.00	0.00	H
ATOM	2374	2HG1	ILE	192	111.620	90.711	78.536	1.00	0.00	H
ATOM	2375	2HG2	ILE	192	109.842	90.969	82.524	1.00	0.00	H
ATOM	2376	3HG2	ILE	192	109.133	89.964	81.241	1.00	0.00	H
ATOM	2377	1HG2	ILE	192	110.648	89.485	82.042	1.00	0.00	H
ATOM	2378	2HD1	ILE	192	113.309	89.619	80.049	1.00	0.00	H
ATOM	2379	3HD1	ILE	192	112.073	88.451	80.588	1.00	0.00	H
ATOM	2380	1HD1	ILE	192	112.580	88.482	78.887	1.00	0.00	H
ATOM	2381	N	GLY	193	108.501	93.593	81.560	1.00	0.00	N
ATOM	2382	CA	GLY	193	107.981	94.465	82.644	1.00	0.00	C
ATOM	2383	C	GLY	193	106.797	93.807	83.394	1.00	0.00	C
ATOM	2384	O	GLY	193	106.069	92.963	82.867	1.00	0.00	O
ATOM	2385	H	GLY	193	107.857	92.935	81.093	1.00	0.00	H
ATOM	2386	1HA	GLY	193	108.780	94.742	83.361	1.00	0.00	H

ATOM	2387	2HA	GLY	193	107.620	95.417	82.214	1.00	0.00	H
ATOM	2388	N	ASP	194	106.620	94.204	84.651	0.00	0.00	N
ATOM	2389	CA	ASP	194	105.779	93.470	85.637	0.00	0.00	C
ATOM	2390	C	ASP	194	106.338	92.050	86.040	0.00	0.00	C
ATOM	2391	O	ASP	194	106.262	91.059	85.311	0.00	0.00	O
ATOM	2392	CB	ASP	194	104.243	93.694	85.490	0.00	0.00	C
ATOM	2393	CG	ASP	194	103.710	94.969	86.165	0.00	0.00	C
ATOM	2394	OD1	ASP	194	102.591	94.994	86.709	0.00	0.00	O
ATOM	2395	OD2	ASP	194	104.420	95.994	86.207	0.00	0.00	O
ATOM	2396	H	ASP	194	107.243	94.956	84.952	0.00	0.00	H
ATOM	2397	HA	ASP	194	106.000	94.081	86.538	0.00	0.00	H
ATOM	2398	1HB	ASP	194	103.702	92.835	85.929	0.00	0.00	H
ATOM	2399	2HB	ASP	194	103.950	93.706	84.427	0.00	0.00	H
ATOM	2400	N	PHE	195	106.971	92.028	87.220	0.00	0.00	N
ATOM	2401	CA	PHE	195	107.659	90.844	87.809	0.00	0.00	C
ATOM	2402	C	PHE	195	106.955	90.346	89.118	0.00	0.00	C
ATOM	2403	O	PHE	195	107.603	89.677	89.928	0.00	0.00	O
ATOM	2404	CB	PHE	195	109.123	91.329	88.053	0.00	0.00	C
ATOM	2405	CG	PHE	195	110.056	91.346	86.828	0.00	0.00	C
ATOM	2406	CD1	PHE	195	110.856	90.237	86.538	0.00	0.00	C
ATOM	2407	CE1	PHE	195	111.733	90.267	85.457	0.00	0.00	C
ATOM	2408	CZ	PHE	195	111.821	91.406	84.661	0.00	0.00	C
ATOM	2409	CE2	PHE	195	111.028	92.514	84.943	0.00	0.00	C
ATOM	2410	CD2	PHE	195	110.140	92.480	86.015	0.00	0.00	C
ATOM	2411	H	PHE	195	106.824	92.881	87.779	0.00	0.00	H
ATOM	2412	HA	PHE	195	107.709	89.937	87.162	0.00	0.00	H
ATOM	2413	1HB	PHE	195	109.585	90.688	88.817	0.00	0.00	H
ATOM	2414	2HB	PHE	195	109.136	92.321	88.548	0.00	0.00	H
ATOM	2415	HD1	PHE	195	110.792	89.343	87.141	0.00	0.00	H
ATOM	2416	HE1	PHE	195	112.334	89.398	85.231	0.00	0.00	H
ATOM	2417	HZ	PHE	195	112.500	91.427	83.821	0.00	0.00	H
ATOM	2418	HE2	PHE	195	111.092	93.402	84.334	0.00	0.00	H
ATOM	2419	HD2	PHE	195	109.522	93.343	86.222	0.00	0.00	H
ATOM	2420	N	GLY	196	105.650	90.587	89.364	0.00	0.00	N
ATOM	2421	CA	GLY	196	105.014	90.327	90.689	0.00	0.00	C
ATOM	2422	C	GLY	196	104.105	89.088	90.820	0.00	0.00	C
ATOM	2423	O	GLY	196	102.957	89.227	91.239	0.00	0.00	O
ATOM	2424	H	GLY	196	105.226	91.180	88.638	0.00	0.00	H
ATOM	2425	1HA	GLY	196	104.419	91.219	90.959	0.00	0.00	H
ATOM	2426	2HA	GLY	196	105.762	90.262	91.504	0.00	0.00	H
ATOM	2427	N	LEU	197	104.634	87.889	90.543	1.00	0.00	N
ATOM	2428	CA	LEU	197	104.022	86.603	91.006	1.00	0.00	C
ATOM	2429	C	LEU	197	105.151	85.715	91.663	1.00	0.00	C
ATOM	2430	O	LEU	197	105.867	86.202	92.541	1.00	0.00	O
ATOM	2431	CB	LEU	197	103.184	85.943	89.856	1.00	0.00	C
ATOM	2432	CG	LEU	197	101.879	86.642	89.386	1.00	0.00	C
ATOM	2433	CD1	LEU	197	101.258	85.871	88.209	1.00	0.00	C
ATOM	2434	CD2	LEU	197	100.819	86.751	90.496	1.00	0.00	C
ATOM	2435	H	LEU	197	105.635	87.961	90.323	1.00	0.00	H
ATOM	2436	HA	LEU	197	103.337	86.799	91.855	1.00	0.00	H
ATOM	2437	1HB	LEU	197	103.851	85.796	88.985	1.00	0.00	H
ATOM	2438	2HB	LEU	197	102.903	84.921	90.170	1.00	0.00	H
ATOM	2439	HG	LEU	197	102.132	87.665	89.038	1.00	0.00	H
ATOM	2440	2HD1	LEU	197	101.973	85.727	87.381	1.00	0.00	H
ATOM	2441	3HD1	LEU	197	100.903	84.864	88.502	1.00	0.00	H
ATOM	2442	1HD1	LEU	197	100.391	86.412	87.783	1.00	0.00	H
ATOM	2443	2HD2	LEU	197	100.543	85.768	90.917	1.00	0.00	H
ATOM	2444	3HD2	LEU	197	101.167	87.379	91.337	1.00	0.00	H
ATOM	2445	1HD2	LEU	197	99.890	87.324	90.127	1.00	0.00	H
ATOM	2446	N	ALA	198	105.281	84.400	91.365	0.00	0.00	N
ATOM	2447	CA	ALA	198	106.332	83.495	91.954	0.00	0.00	C
ATOM	2448	C	ALA	198	106.887	82.527	90.913	1.00	0.00	C

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ATOM   2460  CB  THR   199     104.846  84.607  96.453  0.00  0.00           C
ATOM   2461  OG1 THR   199     105.108  85.041  97.781  0.00  0.00           O
ATOM   2462  CG2 THR   199     103.621  83.679  96.562  0.00  0.00           C
ATOM   2463  H   THR   199     104.928  83.743  94.023  0.00  0.00           H
ATOM   2464  HA  THR   199     106.844  84.891  95.797  0.00  0.00           H
ATOM   2465  HB  THR   199     104.555  85.498  95.858  0.00  0.00           H
ATOM   2466  HG1 THR   199     105.389  84.253  98.258  0.00  0.00           H
ATOM   2467 1HG2 THR   199     103.274  83.329  95.574  0.00  0.00           H
ATOM   2468 2HG2 THR   199     103.828  82.784  97.176  0.00  0.00           H
ATOM   2469 3HG2 THR   199     102.768  84.204  97.033  0.00  0.00           H
ATOM   2470  N   LYS   200     108.191  82.708  96.444  0.00  0.00           N
ATOM   2471  CA  LYS   200     109.045  81.751  97.211  0.00  0.00           C
ATOM   2472  C   LYS   200     110.269  82.493  97.854  0.00  0.00           C
ATOM   2473  O   LYS   200     110.965  83.267  97.191  0.00  0.00           O
ATOM   2474  CB  LYS   200     109.511  80.590  96.281  0.00  0.00           C
ATOM   2475  CG  LYS   200     108.392  79.733  95.634  0.00  0.00           C
ATOM   2476  CD  LYS   200     108.929  78.488  94.901  0.00  0.00           C
ATOM   2477  CE  LYS   200     107.840  77.788  94.074  0.00  0.00           C
ATOM   2478  NZ  LYS   200     108.399  76.594  93.408  0.00  0.00           N
ATOM   2479 1HZ  LYS   200     107.662  76.132  92.856  1.00  0.00           H
ATOM   2480 2HZ  LYS   200     109.168  76.877  92.784  1.00  0.00           H
ATOM   2481 3HZ  LYS   200     108.757  75.940  94.118  1.00  0.00           H
ATOM   2482  H   LYS   200     108.518  83.167  95.581  0.00  0.00           H
ATOM   2483  HA  LYS   200     108.457  81.285  98.030  0.00  0.00           H
ATOM   2484 1HB  LYS   200     110.160  81.001  95.481  0.00  0.00           H
ATOM   2485 2HB  LYS   200     110.174  79.924  96.865  0.00  0.00           H
ATOM   2486 1HG  LYS   200     107.653  79.425  96.400  0.00  0.00           H
ATOM   2487 2HG  LYS   200     107.826  80.368  94.923  0.00  0.00           H
ATOM   2488 1HD  LYS   200     109.766  78.777  94.234  0.00  0.00           H
ATOM   2489 2HD  LYS   200     109.366  77.785  95.637  0.00  0.00           H
ATOM   2490 1HE  LYS   200     106.978  77.501  94.711  0.00  0.00           H
ATOM   2491 2HE  LYS   200     107.440  78.483  93.308  0.00  0.00           H
ATOM   2492  N   VAL   201     110.533  82.262  99.151  0.00  0.00           N
ATOM   2493  CA  VAL   201     111.582  83.002  99.926  0.00  0.00           C
ATOM   2494  C   VAL   201     112.931  82.205 100.056  0.00  0.00           C
ATOM   2495  O   VAL   201     112.932  80.973 100.172  0.00  0.00           O
ATOM   2496  CB  VAL   201     110.952  83.444 101.300  0.00  0.00           C
ATOM   2497  CG1 VAL   201     110.769  82.319 102.349  0.00  0.00           C
ATOM   2498  CG2 VAL   201     111.719  84.604 101.969  0.00  0.00           C
ATOM   2499  H   VAL   201     109.948  81.547  99.591  0.00  0.00           H
ATOM   2500  HA  VAL   201     111.822  83.938  99.379  0.00  0.00           H
ATOM   2501  HB  VAL   201     109.942  83.850 101.080  0.00  0.00           H
ATOM   2502 1HG1 VAL   201     111.738  81.929 102.713  0.00  0.00           H
ATOM   2503 2HG1 VAL   201     110.206  82.666 103.235  0.00  0.00           H
ATOM   2504 3HG1 VAL   201     110.214  81.455 101.938  0.00  0.00           H
ATOM   2505 1HG2 VAL   201     112.741  84.312 102.280  0.00  0.00           H
ATOM   2506 2HG2 VAL   201     111.820  85.473 101.292  0.00  0.00           H
ATOM   2507 3HG2 VAL   201     111.200  84.973 102.874  0.00  0.00           H
ATOM   2508  N   GLU   202     114.083  82.901 100.125  0.00  0.00           N
ATOM   2509  CA  GLU   202     115.425  82.250 100.286  0.00  0.00           C
ATOM   2510  C   GLU   202     115.779  81.725 101.739  0.00  0.00           C
ATOM   2511  O   GLU   202     116.881  81.934 102.253  0.00  0.00           O
ATOM   2512  CB  GLU   202     116.504  83.217  99.708  0.00  0.00           C
ATOM   2513  CG  GLU   202     116.458  83.535  98.184  0.00  0.00           C
ATOM   2514  CD  GLU   202     115.676  84.788  97.775  0.00  0.00           C
ATOM   2515  OE1 GLU   202     114.539  85.053  98.156  0.00  0.00           O
ATOM   2516  OE2 GLU   202     116.386  85.585  96.932  0.00  0.00           O
ATOM   2517  H   GLU   202     114.001  83.871  99.795  0.00  0.00           H
ATOM   2518  HA  GLU   202     115.455  81.342  99.651  0.00  0.00           H
ATOM   2519 1HB  GLU   202     116.534  84.153 100.302  0.00  0.00           H
ATOM   2520 2HB  GLU   202     117.493  82.758  99.902  0.00  0.00           H
ATOM   2521 1HG  GLU   202     117.496  83.646  97.815  0.00  0.00           H
ATOM   2522 2HG  GLU   202     116.054  82.676  97.616  0.00  0.00           H
ATOM   2523  N   TYR   203     114.863  80.962 102.354  0.00  0.00           N
ATOM   2524  CA  TYR   203     115.139  80.119 103.556  0.00  0.00           C
ATOM   2525  C   TYR   203     114.495  78.695 103.433  0.00  0.00           C
ATOM   2526  O   TYR   203     115.206  77.708 103.643  0.00  0.00           O
ATOM   2527  CB  TYR   203     114.729  80.840 104.875  0.00  0.00           C
ATOM   2528  CG  TYR   203     115.716  81.901 105.398  0.00  0.00           C
ATOM   2529  CD1 TYR   203     116.989  81.520 105.840  0.00  0.00           C
ATOM   2530  CE1 TYR   203     117.875  82.471 106.344  0.00  0.00           C
ATOM   2531  CZ  TYR   203     117.489  83.805 106.423  0.00  0.00           C
ATOM   2532  OH  TYR   203     118.352  84.738 106.929  0.00  0.00           O
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ATOM	2533	CE2	TYR	203	116.225	84.194	105.991	0.00	0.00	C
ATOM	2534	CD2	TYR	203	115.340	83.246	105.477	0.00	0.00	C
ATOM	2535	H	TYR	203	113.907	80.956	101.972	1.00	0.00	H
ATOM	2536	HA	TYR	203	116.228	79.912	103.608	0.00	0.00	H
ATOM	2537	1HB	TYR	203	113.711	81.261	104.769	0.00	0.00	H
ATOM	2538	2HB	TYR	203	114.617	80.092	105.682	0.00	0.00	H
ATOM	2539	HD1	TYR	203	117.300	80.485	105.787	0.00	0.00	H
ATOM	2540	HE1	TYR	203	118.858	82.164	106.672	0.00	0.00	H
ATOM	2541	HH	TYR	203	119.183	84.305	107.133	0.00	0.00	H
ATOM	2542	HE2	TYR	203	115.933	85.231	106.059	0.00	0.00	H
ATOM	2543	HD2	TYR	203	114.361	83.561	105.145	0.00	0.00	H
ATOM	2544	N	ASP	204	113.189	78.546	103.110	0.00	0.00	N
ATOM	2545	CA	ASP	204	112.574	77.215	102.817	0.00	0.00	C
ATOM	2546	C	ASP	204	111.617	77.238	101.564	0.00	0.00	C
ATOM	2547	O	ASP	204	110.886	78.205	101.331	0.00	0.00	O
ATOM	2548	CB	ASP	204	111.973	76.596	104.114	0.00	0.00	C
ATOM	2549	CG	ASP	204	110.524	76.932	104.462	0.00	0.00	C
ATOM	2550	OD1	ASP	204	110.164	77.963	105.017	0.00	0.00	O
ATOM	2551	OD2	ASP	204	109.676	75.937	104.080	0.00	0.00	O
ATOM	2552	H	ASP	204	112.693	79.423	102.920	0.00	0.00	H
ATOM	2553	HA	ASP	204	113.401	76.532	102.528	0.00	0.00	H
ATOM	2554	1HB	ASP	204	112.050	75.497	104.043	0.00	0.00	H
ATOM	2555	2HB	ASP	204	112.599	76.844	104.991	0.00	0.00	H
ATOM	2556	N	GLY	205	111.602	76.142	100.783	0.00	0.00	N
ATOM	2557	CA	GLY	205	110.724	76.006	99.584	0.00	0.00	C
ATOM	2558	C	GLY	205	109.511	75.068	99.784	0.00	0.00	C
ATOM	2559	O	GLY	205	109.682	73.872	100.024	0.00	0.00	O
ATOM	2560	H	GLY	205	112.181	75.370	101.128	0.00	0.00	H
ATOM	2561	1HA	GLY	205	110.407	76.994	99.196	0.00	0.00	H
ATOM	2562	2HA	GLY	205	111.323	75.579	98.760	0.00	0.00	H
ATOM	2563	N	GLU	206	108.290	75.605	99.660	0.00	0.00	N
ATOM	2564	CA	GLU	206	107.034	74.858	99.972	0.00	0.00	C
ATOM	2565	C	GLU	206	105.858	75.267	99.020	0.00	0.00	C
ATOM	2566	O	GLU	206	105.527	76.451	98.906	0.00	0.00	O
ATOM	2567	CB	GLU	206	106.695	75.043	101.487	0.00	0.00	C
ATOM	2568	CG	GLU	206	106.381	76.487	101.985	0.00	0.00	C
ATOM	2569	CD	GLU	206	106.297	76.676	103.499	0.00	0.00	C
ATOM	2570	OE1	GLU	206	107.039	76.129	104.309	0.00	0.00	O
ATOM	2571	OE2	GLU	206	105.335	77.567	103.853	0.00	0.00	O
ATOM	2572	H	GLU	206	108.289	76.621	99.527	0.00	0.00	H
ATOM	2573	HA	GLU	206	107.213	73.774	99.821	0.00	0.00	H
ATOM	2574	1HB	GLU	206	105.848	74.381	101.750	0.00	0.00	H
ATOM	2575	2HB	GLU	206	107.545	74.637	102.075	0.00	0.00	H
ATOM	2576	1HG	GLU	206	107.156	77.189	101.629	0.00	0.00	H
ATOM	2577	2HG	GLU	206	105.439	76.843	101.526	0.00	0.00	H
ATOM	2578	N	ARG	207	105.178	74.299	98.371	0.00	0.00	N
ATOM	2579	CA	ARG	207	103.984	74.593	97.511	0.00	0.00	C
ATOM	2580	C	ARG	207	102.644	74.622	98.338	0.00	0.00	C
ATOM	2581	O	ARG	207	101.731	73.817	98.148	0.00	0.00	O
ATOM	2582	CB	ARG	207	103.948	73.615	96.295	0.00	0.00	C
ATOM	2583	CG	ARG	207	105.115	73.695	95.268	0.00	0.00	C
ATOM	2584	CD	ARG	207	106.268	72.718	95.557	0.00	0.00	C
ATOM	2585	NE	ARG	207	107.373	72.962	94.591	0.00	0.00	N
ATOM	2586	CZ	ARG	207	108.655	73.134	94.889	0.00	0.00	C
ATOM	2587	NH1	ARG	207	109.140	73.144	96.096	0.00	0.00	N
ATOM	2588	NH2	ARG	207	109.474	73.306	93.911	0.00	0.00	N
ATOM	2589	HE	ARG	207	107.118	73.002	93.594	1.00	0.00	H
ATOM	2590	H	ARG	207	105.521	73.344	98.513	0.00	0.00	H
ATOM	2591	HA	ARG	207	104.084	75.202	97.063	0.00	0.00	H
ATOM	2592	1HB	ARG	207	103.801	73.574	96.640	0.00	0.00	H
ATOM	2593	2HB	ARG	207	103.015	73.828	95.772	0.00	0.00	H
ATOM	2594	1HG	ARG	207	104.771	73.131	94.887	0.00	0.00	H

ATOM	2606	CB	LYS	208	102.023	76.067	101.541	0.00	0.00	C
ATOM	2607	CG	LYS	208	101.078	76.180	102.758	0.00	0.00	C
ATOM	2608	CD	LYS	208	101.870	76.109	104.081	0.00	0.00	C
ATOM	2609	CE	LYS	208	101.036	76.510	105.304	0.00	0.00	C
ATOM	2610	NZ	LYS	208	101.838	76.307	106.527	0.00	0.00	N
ATOM	2611	1HZ	LYS	208	101.282	76.576	107.351	1.00	0.00	H
ATOM	2612	2HZ	LYS	208	102.106	75.315	106.602	1.00	0.00	H
ATOM	2613	3HZ	LYS	208	102.687	76.889	106.482	1.00	0.00	H
ATOM	2614	H	LYS	208	103.435	76.102	99.387	0.00	0.00	H
ATOM	2615	HA	LYS	208	100.792	74.856	100.241	0.00	0.00	H
ATOM	2616	1HB	LYS	208	102.739	75.245	101.756	0.00	0.00	H
ATOM	2617	2HB	LYS	208	102.644	76.983	101.497	0.00	0.00	H
ATOM	2618	1HG	LYS	208	100.505	77.126	102.695	0.00	0.00	H
ATOM	2619	2HG	LYS	208	100.318	75.374	102.740	0.00	0.00	H
ATOM	2620	1HD	LYS	208	102.260	75.079	104.211	0.00	0.00	H
ATOM	2621	2HD	LYS	208	102.765	76.757	104.020	0.00	0.00	H
ATOM	2622	1HE	LYS	208	100.722	77.570	105.221	0.00	0.00	H
ATOM	2623	2HE	LYS	208	100.104	75.914	105.360	0.00	0.00	H
ATOM	2624	N	LYS	209	100.659	77.740	98.691	0.00	0.00	N
ATOM	2625	CA	LYS	209	99.705	78.666	97.997	0.00	0.00	C
ATOM	2626	C	LYS	209	99.374	78.284	96.498	0.00	0.00	C
ATOM	2627	O	LYS	209	98.226	78.420	96.065	0.00	0.00	O
ATOM	2628	CB	LYS	209	100.265	80.104	98.203	0.00	0.00	C
ATOM	2629	CG	LYS	209	99.332	81.261	97.765	0.00	0.00	C
ATOM	2630	CD	LYS	209	99.630	81.806	96.350	0.00	0.00	C
ATOM	2631	CE	LYS	209	98.518	82.713	95.793	0.00	0.00	C
ATOM	2632	NZ	LYS	209	97.422	81.903	95.221	0.00	0.00	N
ATOM	2633	1HZ	LYS	209	96.689	82.527	94.854	1.00	0.00	H
ATOM	2634	2HZ	LYS	209	97.789	81.319	94.457	1.00	0.00	H
ATOM	2635	3HZ	LYS	209	97.023	81.299	95.954	1.00	0.00	H
ATOM	2636	H	LYS	209	101.624	77.598	98.384	0.00	0.00	H
ATOM	2637	HA	LYS	209	98.723	78.635	98.513	0.00	0.00	H
ATOM	2638	1HB	LYS	209	100.457	80.245	99.286	0.00	0.00	H
ATOM	2639	2HB	LYS	209	101.263	80.211	97.735	0.00	0.00	H
ATOM	2640	1HG	LYS	209	98.273	80.948	97.853	0.00	0.00	H
ATOM	2641	2HG	LYS	209	99.430	82.095	98.485	0.00	0.00	H
ATOM	2642	1HD	LYS	209	100.572	82.388	96.396	0.00	0.00	H
ATOM	2643	2HD	LYS	209	99.846	80.986	95.638	0.00	0.00	H
ATOM	2644	1HE	LYS	209	98.125	83.390	96.578	0.00	0.00	H
ATOM	2645	2HE	LYS	209	98.924	83.383	95.009	0.00	0.00	H
ATOM	2646	N	THR	210	100.341	77.767	95.710	0.00	0.00	N
ATOM	2647	CA	THR	210	100.077	76.742	94.640	0.00	0.00	C
ATOM	2648	C	THR	210	99.851	77.267	93.177	0.00	0.00	C
ATOM	2649	O	THR	210	100.677	76.956	92.318	0.00	0.00	O
ATOM	2650	CB	THR	210	99.149	75.559	95.084	0.00	0.00	C
ATOM	2651	OG1	THR	210	99.601	75.041	96.330	0.00	0.00	O
ATOM	2652	CG2	THR	210	99.114	74.344	94.145	0.00	0.00	C
ATOM	2653	H	THR	210	101.215	77.717	96.237	0.00	0.00	H
ATOM	2654	HA	THR	210	101.060	76.239	94.553	0.00	0.00	H
ATOM	2655	HB	THR	210	98.116	75.943	95.207	0.00	0.00	H
ATOM	2656	HG1	THR	210	99.191	74.178	96.440	0.00	0.00	H
ATOM	2657	1HG2	THR	210	98.450	73.553	94.537	0.00	0.00	H
ATOM	2658	2HG2	THR	210	98.737	74.606	93.138	0.00	0.00	H
ATOM	2659	3HG2	THR	210	100.117	73.895	94.010	0.00	0.00	H
ATOM	2660	N	LEU	211	98.760	77.989	92.859	0.00	0.00	N
ATOM	2661	CA	LEU	211	98.390	78.383	91.462	0.00	0.00	C
ATOM	2662	C	LEU	211	98.152	79.921	91.268	0.00	0.00	C
ATOM	2663	O	LEU	211	97.299	80.524	91.926	0.00	0.00	O
ATOM	2664	CB	LEU	211	97.152	77.525	91.055	0.00	0.00	C
ATOM	2665	CG	LEU	211	96.653	77.648	89.589	0.00	0.00	C
ATOM	2666	CD1	LEU	211	97.684	77.137	88.570	0.00	0.00	C
ATOM	2667	CD2	LEU	211	95.344	76.862	89.403	0.00	0.00	C
ATOM	2668	H	LEU	211	98.174	78.215	93.673	1.00	0.00	H
ATOM	2669	HA	LEU	211	99.205	78.082	90.775	0.00	0.00	H
ATOM	2670	1HB	LEU	211	96.317	77.777	91.739	0.00	0.00	H
ATOM	2671	2HB	LEU	211	97.367	76.457	91.258	0.00	0.00	H
ATOM	2672	HG	LEU	211	96.437	78.714	89.370	0.00	0.00	H
ATOM	2673	1HD1	LEU	211	97.305	77.209	87.538	0.00	0.00	H
ATOM	2674	2HD1	LEU	211	98.623	77.717	88.593	0.00	0.00	H
ATOM	2675	3HD1	LEU	211	97.946	76.077	88.745	0.00	0.00	H
ATOM	2676	1HD2	LEU	211	94.944	76.959	88.377	0.00	0.00	H
ATOM	2677	2HD2	LEU	211	95.475	75.781	89.600	0.00	0.00	H
ATOM	2678	3HD2	LEU	211	94.551	77.222	90.084	0.00	0.00	H

ATOM	2679	N	CYS	212	98.844	80.530	90.287	0.00	0.00	N
ATOM	2680	CA	CYS	212	98.480	81.859	89.721	0.00	0.00	C
ATOM	2681	C	CYS	212	98.878	82.007	88.209	0.00	0.00	C
ATOM	2682	O	CYS	212	99.672	81.234	87.662	0.00	0.00	O
ATOM	2683	CB	CYS	212	99.121	82.952	90.615	0.00	0.00	C
ATOM	2684	SG	CYS	212	100.943	82.953	90.479	0.00	0.00	S
ATOM	2685	H	CYS	212	99.566	79.952	89.843	0.00	0.00	H
ATOM	2686	HA	CYS	212	97.378	81.976	89.772	0.00	0.00	H
ATOM	2687	1HB	CYS	212	98.834	82.823	91.677	0.00	0.00	H
ATOM	2688	2HB	CYS	212	98.750	83.954	90.330	0.00	0.00	H
ATOM	2689	HG	CYS	212	101.154	81.796	91.094	1.00	0.00	H
ATOM	2690	N	GLY	213	98.337	83.037	87.535	0.00	0.00	N
ATOM	2691	CA	GLY	213	98.800	83.453	86.181	0.00	0.00	C
ATOM	2692	C	GLY	213	97.663	83.738	85.183	0.00	0.00	C
ATOM	2693	O	GLY	213	96.866	84.657	85.383	0.00	0.00	O
ATOM	2694	H	GLY	213	97.707	83.619	88.099	0.00	0.00	H
ATOM	2695	1HA	GLY	213	99.534	82.740	85.752	0.00	0.00	H
ATOM	2696	2HA	GLY	213	99.374	84.392	86.282	0.00	0.00	H
ATOM	2697	N	THR	214	97.627	82.972	84.088	0.00	0.00	N
ATOM	2698	CA	THR	214	96.718	83.237	82.933	0.00	0.00	C
ATOM	2699	C	THR	214	96.128	81.867	82.441	0.00	0.00	C
ATOM	2700	O	THR	214	96.917	81.060	81.936	0.00	0.00	O
ATOM	2701	CB	THR	214	97.505	83.999	81.819	0.00	0.00	C
ATOM	2702	OG1	THR	214	97.923	85.263	82.313	0.00	0.00	O
ATOM	2703	CG2	THR	214	96.715	84.308	80.537	0.00	0.00	C
ATOM	2704	H	THR	214	98.341	82.239	84.062	0.00	0.00	H
ATOM	2705	HA	THR	214	95.895	83.909	83.235	0.00	0.00	H
ATOM	2706	HB	THR	214	98.407	83.413	81.557	0.00	0.00	H
ATOM	2707	HG1	THR	214	98.390	85.696	81.594	0.00	0.00	H
ATOM	2708	1HG2	THR	214	97.329	84.855	79.799	0.00	0.00	H
ATOM	2709	2HG2	THR	214	96.367	83.386	80.036	0.00	0.00	H
ATOM	2710	3HG2	THR	214	95.823	84.928	80.747	0.00	0.00	H
ATOM	2711	N	PRO	215	94.799	81.546	82.525	0.00	0.00	N
ATOM	2712	CA	PRO	215	94.254	80.205	82.148	0.00	0.00	C
ATOM	2713	CD	PRO	215	93.794	82.405	83.185	0.00	0.00	C
ATOM	2714	C	PRO	215	94.668	79.504	80.814	0.00	0.00	C
ATOM	2715	O	PRO	215	94.961	78.311	80.835	0.00	0.00	O
ATOM	2716	CB	PRO	215	92.735	80.418	82.290	0.00	0.00	C
ATOM	2717	CG	PRO	215	92.599	81.474	83.388	0.00	0.00	C
ATOM	2718	HA	PRO	215	94.580	79.510	82.945	0.00	0.00	H
ATOM	2719	1HD	PRO	215	93.527	83.261	82.535	0.00	0.00	H
ATOM	2720	2HD	PRO	215	94.140	82.814	84.156	0.00	0.00	H
ATOM	2721	1HB	PRO	215	92.203	79.478	82.536	0.00	0.00	H
ATOM	2722	2HB	PRO	215	92.296	80.791	81.344	0.00	0.00	H
ATOM	2723	1HG	PRO	215	92.052	80.997	84.386	0.00	0.00	H
ATOM	2724	2HG	PRO	215	91.637	82.017	83.344	0.00	0.00	H
ATOM	2725	N	ASN	216	94.745	80.230	79.689	1.00	0.00	N
ATOM	2726	CA	ASN	216	95.298	79.690	78.401	1.00	0.00	C
ATOM	2727	C	ASN	216	96.866	79.462	78.324	1.00	0.00	C
ATOM	2728	O	ASN	216	97.340	78.817	77.387	1.00	0.00	O
ATOM	2729	CB	ASN	216	94.840	80.631	77.244	1.00	0.00	C
ATOM	2730	CG	ASN	216	93.338	80.908	77.057	1.00	0.00	C
ATOM	2731	OD1	ASN	216	92.446	80.174	77.461	1.00	0.00	O
ATOM	2732	ND2	ASN	216	92.998	82.007	76.437	1.00	0.00	N
ATOM	2733	H	ASN	216	94.425	81.195	79.805	1.00	0.00	H
ATOM	2734	HA	ASN	216	94.848	78.695	78.209	1.00	0.00	H
ATOM	2735	1HB	ASN	216	95.381	81.591	77.334	1.00	0.00	H
ATOM	2736	2HB	ASN	216	95.186	80.193	76.288	1.00	0.00	H
ATOM	2737	1HD2	ASN	216	91.991	82.076	76.364	1.00	0.00	H
ATOM	2738	2HD2	ASN	216	93.751	82.524	75.978	1.00	0.00	H
ATOM	2739	N	TYR	217	97.665	80.015	79.253	0.00	0.00	N
ATOM	2740	CA	TYR	217	99.153	[illegible]	79.205	0.00	0.00	C
[illegible]										

ATOM	2752	HA	TYR	217	99.528	79.534	78.286	0.00	0.00	H
ATOM	2753	1HB	TYR	217	100.632	81.524	79.806	0.00	0.00	H
ATOM	2754	2HB	TYR	217	99.005	82.062	79.960	0.00	0.00	H
ATOM	2755	HD1	TYR	217	101.934	82.173	77.953	0.00	0.00	H
ATOM	2756	HE1	TYR	217	102.158	83.101	75.707	0.00	0.00	H
ATOM	2757	HH	TYR	217	101.054	83.350	73.772	0.00	0.00	H
ATOM	2758	HE2	TYR	217	97.896	83.266	75.315	0.00	0.00	H
ATOM	2759	HD2	TYR	217	97.654	82.353	77.596	0.00	0.00	H
ATOM	2760	N	ILE	218	99.176	78.544	81.339	1.00	0.00	N
ATOM	2761	CA	ILE	218	99.789	77.778	82.473	1.00	0.00	C
ATOM	2762	C	ILE	218	100.234	76.315	82.106	1.00	0.00	C
ATOM	2763	O	ILE	218	99.593	75.634	81.302	1.00	0.00	O
ATOM	2764	CB	ILE	218	98.852	77.782	83.741	1.00	0.00	C
ATOM	2765	CG1	ILE	218	97.441	77.159	83.512	1.00	0.00	C
ATOM	2766	CG2	ILE	218	98.755	79.177	84.408	1.00	0.00	C
ATOM	2767	CD1	ILE	218	96.717	76.713	84.792	1.00	0.00	C
ATOM	2768	H	ILE	218	98.162	78.681	81.261	1.00	0.00	H
ATOM	2769	HA	ILE	218	100.713	78.317	82.768	1.00	0.00	H
ATOM	2770	HB	ILE	218	99.357	77.140	84.489	1.00	0.00	H
ATOM	2771	1HG1	ILE	218	96.797	77.850	82.931	1.00	0.00	H
ATOM	2772	2HG1	ILE	218	97.535	76.264	82.866	1.00	0.00	H
ATOM	2773	2HG2	ILE	218	99.752	79.601	84.631	1.00	0.00	H
ATOM	2774	3HG2	ILE	218	98.227	79.903	83.765	1.00	0.00	H
ATOM	2775	1HG2	ILE	218	98.211	79.141	85.371	1.00	0.00	H
ATOM	2776	2HD1	ILE	218	97.360	76.074	85.427	1.00	0.00	H
ATOM	2777	3HD1	ILE	218	96.388	77.571	85.404	1.00	0.00	H
ATOM	2778	1HD1	ILE	218	95.818	76.116	84.556	1.00	0.00	H
ATOM	2779	N	ALA	219	101.320	75.825	82.731	0.00	0.00	N
ATOM	2780	CA	ALA	219	101.841	74.455	82.485	0.00	0.00	C
ATOM	2781	C	ALA	219	101.206	73.307	83.368	0.00	0.00	C
ATOM	2782	O	ALA	219	100.817	73.579	84.511	0.00	0.00	O
ATOM	2783	CB	ALA	219	103.364	74.552	82.711	0.00	0.00	C
ATOM	2784	H	ALA	219	101.770	76.471	83.382	0.00	0.00	H
ATOM	2785	HA	ALA	219	101.687	74.215	81.416	0.00	0.00	H
ATOM	2786	1HB	ALA	219	103.872	73.623	82.397	0.00	0.00	H
ATOM	2787	2HB	ALA	219	103.825	75.369	82.126	0.00	0.00	H
ATOM	2788	3HB	ALA	219	103.616	74.720	83.775	0.00	0.00	H
ATOM	2789	N	PRO	220	101.158	72.005	82.943	0.00	0.00	N
ATOM	2790	CA	PRO	220	100.659	70.877	83.791	0.00	0.00	C
ATOM	2791	CD	PRO	220	101.394	71.597	81.543	0.00	0.00	C
ATOM	2792	C	PRO	220	101.187	70.651	85.247	0.00	0.00	C
ATOM	2793	O	PRO	220	100.407	70.199	86.082	0.00	0.00	O
ATOM	2794	CB	PRO	220	100.904	69.656	82.883	0.00	0.00	C
ATOM	2795	CG	PRO	220	100.785	70.200	81.462	0.00	0.00	C
ATOM	2796	HA	PRO	220	99.562	71.009	83.886	0.00	0.00	H
ATOM	2797	1HD	PRO	220	102.476	71.581	81.306	0.00	0.00	H
ATOM	2798	2HD	PRO	220	100.898	72.264	80.814	0.00	0.00	H
ATOM	2799	1HB	PRO	220	100.186	68.836	83.080	0.00	0.00	H
ATOM	2800	2HB	PRO	220	101.916	69.231	83.038	0.00	0.00	H
ATOM	2801	1HG	PRO	220	99.721	70.265	81.158	0.00	0.00	H
ATOM	2802	2HG	PRO	220	101.288	69.563	80.711	0.00	0.00	H
ATOM	2803	N	GLU	221	102.455	70.966	85.580	0.00	0.00	N
ATOM	2804	CA	GLU	221	102.945	70.910	86.995	0.00	0.00	C
ATOM	2805	C	GLU	221	102.260	71.890	88.015	0.00	0.00	C
ATOM	2806	O	GLU	221	101.936	71.471	89.129	0.00	0.00	O
ATOM	2807	CB	GLU	221	104.487	71.081	87.071	0.00	0.00	C
ATOM	2808	CG	GLU	221	105.359	69.952	86.464	0.00	0.00	C
ATOM	2809	CD	GLU	221	106.798	70.025	86.972	0.00	0.00	C
ATOM	2810	OE1	GLU	221	107.633	70.826	86.560	0.00	0.00	O
ATOM	2811	OE2	GLU	221	107.020	69.153	87.992	0.00	0.00	O
ATOM	2812	H	GLU	221	102.987	71.365	84.803	0.00	0.00	H
ATOM	2813	HA	GLU	221	102.712	69.898	87.380	0.00	0.00	H
ATOM	2814	1HB	GLU	221	104.749	71.155	88.147	0.00	0.00	H
ATOM	2815	2HB	GLU	221	104.783	72.059	86.645	0.00	0.00	H
ATOM	2816	1HG	GLU	221	105.363	70.002	85.361	0.00	0.00	H
ATOM	2817	2HG	GLU	221	104.941	68.959	86.717	0.00	0.00	H
ATOM	2818	N	VAL	222	102.046	73.170	87.658	1.00	0.00	N
ATOM	2819	CA	VAL	222	101.206	74.108	88.480	1.00	0.00	C
ATOM	2820	C	VAL	222	99.684	73.725	88.570	1.00	0.00	C
ATOM	2821	O	VAL	222	99.093	73.815	89.649	1.00	0.00	O
ATOM	2822	CB	VAL	222	101.425	75.616	88.090	1.00	0.00	C
ATOM	2823	CG1	VAL	222	102.863	76.109	88.353	1.00	0.00	C
ATOM	2824	CG2	VAL	222	101.043	76.020	86.649	1.00	0.00	C

ATOM	2825	H	VAL	222	102.203	73.339	86.661	1.00	0.00	H
ATOM	2826	HA	VAL	222	101.561	74.024	89.528	1.00	0.00	H
ATOM	2827	HB	VAL	222	100.774	76.205	88.767	1.00	0.00	H
ATOM	2828	1HG1	VAL	222	103.609	75.553	87.759	1.00	0.00	H
ATOM	2829	2HG1	VAL	222	102.997	77.183	88.122	1.00	0.00	H
ATOM	2830	3HG1	VAL	222	103.135	75.982	89.416	1.00	0.00	H
ATOM	2831	2HG2	VAL	222	100.005	75.734	86.400	1.00	0.00	H
ATOM	2832	3HG2	VAL	222	101.111	77.114	86.497	1.00	0.00	H
ATOM	2833	1HG2	VAL	222	101.699	75.546	85.896	1.00	0.00	H
ATOM	2834	N	LEU	223	99.058	73.284	87.463	1.00	0.00	N
ATOM	2835	CA	LEU	223	97.660	72.767	87.463	1.00	0.00	C
ATOM	2836	C	LEU	223	97.419	71.428	88.252	1.00	0.00	C
ATOM	2837	O	LEU	223	96.535	71.382	89.110	1.00	0.00	O
ATOM	2838	CB	LEU	223	97.223	72.719	85.970	1.00	0.00	C
ATOM	2839	CG	LEU	223	95.765	72.282	85.690	1.00	0.00	C
ATOM	2840	CD1	LEU	223	94.728	73.218	86.333	1.00	0.00	C
ATOM	2841	CD2	LEU	223	95.530	72.202	84.175	1.00	0.00	C
ATOM	2842	H	LEU	223	99.671	73.215	86.643	1.00	0.00	H
ATOM	2843	HA	LEU	223	97.031	73.525	87.968	1.00	0.00	H
ATOM	2844	1HB	LEU	223	97.391	73.708	85.502	1.00	0.00	H
ATOM	2845	2HB	LEU	223	97.903	72.033	85.428	1.00	0.00	H
ATOM	2846	HG	LEU	223	95.616	71.263	86.104	1.00	0.00	H
ATOM	2847	2HD1	LEU	223	94.851	73.284	87.429	1.00	0.00	H
ATOM	2848	3HD1	LEU	223	94.782	74.249	85.935	1.00	0.00	H
ATOM	2849	1HD1	LEU	223	93.699	72.854	86.179	1.00	0.00	H
ATOM	2850	2HD2	LEU	223	95.604	73.188	83.680	1.00	0.00	H
ATOM	2851	3HD2	LEU	223	96.256	71.532	83.677	1.00	0.00	H
ATOM	2852	1HD2	LEU	223	94.532	71.792	83.951	1.00	0.00	H
ATOM	2853	N	SER	224	98.187	70.356	87.989	1.00	0.00	N
ATOM	2854	CA	SER	224	98.075	69.064	88.736	1.00	0.00	C
ATOM	2855	C	SER	224	98.658	68.999	90.199	1.00	0.00	C
ATOM	2856	O	SER	224	98.658	67.921	90.799	1.00	0.00	O
ATOM	2857	CB	SER	224	98.741	67.985	87.840	1.00	0.00	C
ATOM	2858	OG	SER	224	98.135	67.870	86.550	1.00	0.00	O
ATOM	2859	H	SER	224	98.879	70.476	87.238	1.00	0.00	H
ATOM	2860	HA	SER	224	97.005	68.795	88.832	1.00	0.00	H
ATOM	2861	1HB	SER	224	99.820	68.204	87.720	1.00	0.00	H
ATOM	2862	2HB	SER	224	98.702	66.998	88.340	1.00	0.00	H
ATOM	2863	HG	SER	224	97.378	67.267	86.625	1.00	0.00	H
ATOM	2864	N	LYS	225	99.135	70.118	90.782	1.00	0.00	N
ATOM	2865	CA	LYS	225	99.694	70.188	92.172	1.00	0.00	C
ATOM	2866	C	LYS	225	101.005	69.347	92.400	1.00	0.00	C
ATOM	2867	O	LYS	225	101.078	68.465	93.259	1.00	0.00	O
ATOM	2868	CB	LYS	225	98.586	69.988	93.255	1.00	0.00	C
ATOM	2869	CG	LYS	225	97.368	70.940	93.162	1.00	0.00	C
ATOM	2870	CD	LYS	225	96.400	70.792	94.350	1.00	0.00	C
ATOM	2871	CE	LYS	225	95.179	71.713	94.203	1.00	0.00	C
ATOM	2872	NZ	LYS	225	94.285	71.539	95.364	1.00	0.00	N
ATOM	2873	1HZ	LYS	225	93.467	72.156	95.264	1.00	0.00	H
ATOM	2874	2HZ	LYS	225	93.970	70.559	95.412	1.00	0.00	H
ATOM	2875	3HZ	LYS	225	94.792	71.779	96.228	1.00	0.00	H
ATOM	2876	H	LYS	225	98.995	70.950	90.199	1.00	0.00	H
ATOM	2877	HA	LYS	225	100.027	71.236	92.303	1.00	0.00	H
ATOM	2878	1HB	LYS	225	98.236	68.938	93.219	1.00	0.00	H
ATOM	2879	2HB	LYS	225	99.054	70.093	94.253	1.00	0.00	H
ATOM	2880	1HG	LYS	225	97.711	71.987	93.077	1.00	0.00	H
ATOM	2881	2HG	LYS	225	96.921	70.743	92.216	1.00	0.00	H
ATOM	2882	1HD	LYS	225	96.066	69.738	94.425	1.00	0.00	H
ATOM	2883	2HD	LYS	225	96.934	71.007	95.295	1.00	0.00	H
ATOM	2884	1HE	LYS	225	95.494	72.772	94.114	1.00	0.00	H
ATOM	2885	2HE	LYS	225	94.630	71.475	93.268	1.00	0.00	H
ATOM	2886	N	LYS	226	102.051	69.678	92.213	1.00	0.00	N

ATOM	2898	H	LYS	226	101.835	70.349	90.892	0.00	0.00	H
ATOM	2899	HA	LYS	226	103.295	68.031	92.309	0.00	0.00	H
ATOM	2900	1HB	LYS	226	104.478	67.911	89.973	0.00	0.00	H
ATOM	2901	2HB	LYS	226	103.337	69.102	89.410	0.00	0.00	H
ATOM	2902	1HG	LYS	226	101.442	67.407	90.074	0.00	0.00	H
ATOM	2903	2HG	LYS	226	102.712	66.247	90.442	0.00	0.00	H
ATOM	2904	1HD	LYS	226	103.564	66.527	88.001	0.00	0.00	H
ATOM	2905	2HD	LYS	226	102.191	67.603	87.712	0.00	0.00	H
ATOM	2906	1HE	LYS	226	100.625	65.645	88.456	0.00	0.00	H
ATOM	2907	2HE	LYS	226	102.050	64.607	88.504	0.00	0.00	H
ATOM	2908	N	GLY	227	105.779	69.164	92.013	0.00	0.00	N
ATOM	2909	CA	GLY	227	107.043	69.942	92.196	0.00	0.00	C
ATOM	2910	C	GLY	227	107.474	70.781	90.969	0.00	0.00	C
ATOM	2911	O	GLY	227	108.252	70.317	90.129	0.00	0.00	O
ATOM	2912	H	GLY	227	105.763	68.170	91.767	0.00	0.00	H
ATOM	2913	1HA	GLY	227	107.867	69.245	92.430	0.00	0.00	H
ATOM	2914	2HA	GLY	227	106.975	70.593	93.090	0.00	0.00	H
ATOM	2915	N	HIS	228	106.938	72.001	90.862	1.00	0.00	N
ATOM	2916	CA	HIS	228	107.134	72.882	89.682	1.00	0.00	C
ATOM	2917	C	HIS	228	108.488	73.673	89.671	1.00	0.00	C
ATOM	2918	O	HIS	228	109.095	73.931	90.713	1.00	0.00	O
ATOM	2919	CB	HIS	228	105.849	73.745	89.522	1.00	0.00	C
ATOM	2920	CG	HIS	228	105.638	74.923	90.476	1.00	0.00	C
ATOM	2921	ND1	HIS	228	104.839	74.852	91.605	1.00	0.00	N
ATOM	2922	CE1	HIS	228	104.822	76.176	91.952	1.00	0.00	C
ATOM	2923	NE2	HIS	228	105.504	77.090	91.195	1.00	0.00	N
ATOM	2924	CD2	HIS	228	106.028	76.252	90.228	1.00	0.00	C
ATOM	2925	H	HIS	228	106.269	72.229	91.611	1.00	0.00	H
ATOM	2926	HA	HIS	228	107.156	72.227	88.789	1.00	0.00	H
ATOM	2927	1HB	HIS	228	105.814	74.126	88.490	1.00	0.00	H
ATOM	2928	2HB	HIS	228	104.952	73.095	89.578	1.00	0.00	H
ATOM	2929	HE1	HIS	228	104.223	76.496	92.796	1.00	0.00	H
ATOM	2930	HE2	HIS	228	105.433	78.113	91.204	1.00	0.00	H
ATOM	2931	HD2	HIS	228	106.583	76.576	89.357	1.00	0.00	H
ATOM	2932	N	SER	229	108.982	74.034	88.477	1.00	0.00	N
ATOM	2933	CA	SER	229	110.344	74.627	88.307	1.00	0.00	C
ATOM	2934	C	SER	229	110.413	75.767	87.228	1.00	0.00	C
ATOM	2935	O	SER	229	109.414	76.160	86.618	1.00	0.00	O
ATOM	2936	CB	SER	229	111.307	73.436	88.019	1.00	0.00	C
ATOM	2937	OG	SER	229	111.082	72.858	86.728	1.00	0.00	O
ATOM	2938	H	SER	229	108.401	73.777	87.675	1.00	0.00	H
ATOM	2939	HA	SER	229	110.667	75.107	89.254	1.00	0.00	H
ATOM	2940	1HB	SER	229	112.359	73.774	88.078	1.00	0.00	H
ATOM	2941	2HB	SER	229	111.226	72.659	88.807	1.00	0.00	H
ATOM	2942	HG	SER	229	110.404	72.178	86.829	1.00	0.00	H
ATOM	2943	N	PHE	230	111.629	76.267	86.950	1.00	0.00	N
ATOM	2944	CA	PHE	230	111.937	77.099	85.741	1.00	0.00	C
ATOM	2945	C	PHE	230	111.471	76.593	84.316	1.00	0.00	C
ATOM	2946	O	PHE	230	111.222	77.406	83.423	1.00	0.00	O
ATOM	2947	CB	PHE	230	113.452	77.459	85.816	1.00	0.00	C
ATOM	2948	CG	PHE	230	114.486	76.333	85.620	1.00	0.00	C
ATOM	2949	CD1	PHE	230	114.974	76.051	84.343	1.00	0.00	C
ATOM	2950	CE1	PHE	230	115.897	75.025	84.148	1.00	0.00	C
ATOM	2951	CZ	PHE	230	116.347	74.284	85.237	1.00	0.00	C
ATOM	2952	CE2	PHE	230	115.881	74.568	86.518	1.00	0.00	C
ATOM	2953	CD2	PHE	230	114.956	75.593	86.710	1.00	0.00	C
ATOM	2954	H	PHE	230	112.386	75.821	87.479	1.00	0.00	H
ATOM	2955	HA	PHE	230	111.391	78.053	85.871	1.00	0.00	H
ATOM	2956	1HB	PHE	230	113.651	78.247	85.071	1.00	0.00	H
ATOM	2957	2HB	PHE	230	113.669	77.979	86.769	1.00	0.00	H
ATOM	2958	HD1	PHE	230	114.632	76.633	83.501	1.00	0.00	H
ATOM	2959	HE1	PHE	230	116.265	74.805	83.156	1.00	0.00	H
ATOM	2960	HZ	PHE	230	117.066	73.490	85.087	1.00	0.00	H
ATOM	2961	HE2	PHE	230	116.243	73.999	87.361	1.00	0.00	H
ATOM	2962	HD2	PHE	230	114.613	75.812	87.710	1.00	0.00	H
ATOM	2963	N	GLU	231	111.292	75.272	84.131	1.00	0.00	N
ATOM	2964	CA	GLU	231	110.562	74.677	82.969	1.00	0.00	C
ATOM	2965	C	GLU	231	109.060	75.098	82.737	1.00	0.00	C
ATOM	2966	O	GLU	231	108.584	75.005	81.604	1.00	0.00	O
ATOM	2967	CB	GLU	231	110.656	73.133	83.100	1.00	0.00	C
ATOM	2968	CG	GLU	231	112.078	72.518	83.008	1.00	0.00	C
ATOM	2969	CD	GLU	231	112.065	70.999	82.925	1.00	0.00	C
ATOM	2970	OE1	GLU	231	112.137	70.254	83.897	1.00	0.00	O

ATOM	2971	OE2	GLU	231	111.937	70.573	81.644	1.00	0.00	O
ATOM	2972	H	GLU	231	111.571	74.703	84.940	1.00	0.00	H
ATOM	2973	HA	GLU	231	111.097	74.967	82.041	1.00	0.00	H
ATOM	2974	1HB	GLU	231	110.167	72.799	84.038	1.00	0.00	H
ATOM	2975	2HB	GLU	231	110.045	72.676	82.297	1.00	0.00	H
ATOM	2976	1HG	GLU	231	112.608	72.906	82.120	1.00	0.00	H
ATOM	2977	2HG	GLU	231	112.696	72.813	83.876	1.00	0.00	H
ATOM	2978	N	VAL	232	108.315	75.563	83.762	0.00	0.00	N
ATOM	2979	CA	VAL	232	106.975	76.233	83.587	0.00	0.00	C
ATOM	2980	C	VAL	232	106.973	77.440	82.572	0.00	0.00	C
ATOM	2981	O	VAL	232	106.066	77.540	81.743	0.00	0.00	O
ATOM	2982	CB	VAL	232	106.397	76.618	85.002	0.00	0.00	C
ATOM	2983	CG1	VAL	232	105.069	77.417	84.983	0.00	0.00	C
ATOM	2984	CG2	VAL	232	106.142	75.406	85.927	0.00	0.00	C
ATOM	2985	H	VAL	232	108.833	75.616	84.649	0.00	0.00	H
ATOM	2986	HA	VAL	232	106.286	75.487	83.145	0.00	0.00	H
ATOM	2987	HB	VAL	232	107.150	77.263	85.501	0.00	0.00	H
ATOM	2988	1HG1	VAL	232	104.717	77.675	86.001	0.00	0.00	H
ATOM	2989	2HG1	VAL	232	105.171	78.380	84.448	0.00	0.00	H
ATOM	2990	3HG1	VAL	232	104.250	76.866	84.487	0.00	0.00	H
ATOM	2991	1HG2	VAL	232	105.825	75.734	86.933	0.00	0.00	H
ATOM	2992	2HG2	VAL	232	105.361	74.727	85.535	0.00	0.00	H
ATOM	2993	3HG2	VAL	232	107.054	74.800	86.076	0.00	0.00	H
ATOM	2994	N	ASP	233	107.988	78.323	82.624	0.00	0.00	N
ATOM	2995	CA	ASP	233	108.152	79.450	81.659	0.00	0.00	C
ATOM	2996	C	ASP	233	108.270	79.073	80.140	0.00	0.00	C
ATOM	2997	O	ASP	233	107.709	79.791	79.312	0.00	0.00	O
ATOM	2998	CB	ASP	233	109.365	80.306	82.112	0.00	0.00	C
ATOM	2999	CG	ASP	233	109.178	81.054	83.429	0.00	0.00	C
ATOM	3000	OD1	ASP	233	108.462	82.039	83.552	0.00	0.00	O
ATOM	3001	OD2	ASP	233	109.888	80.506	84.452	0.00	0.00	O
ATOM	3002	H	ASP	233	108.728	78.048	83.281	0.00	0.00	H
ATOM	3003	HA	ASP	233	107.242	80.084	81.725	0.00	0.00	H
ATOM	3004	1HB	ASP	233	109.579	81.077	81.350	0.00	0.00	H
ATOM	3005	2HB	ASP	233	110.280	79.686	82.156	0.00	0.00	H
ATOM	3006	N	VAL	234	108.966	77.984	79.753	1.00	0.00	N
ATOM	3007	CA	VAL	234	109.051	77.551	78.315	1.00	0.00	C
ATOM	3008	C	VAL	234	107.716	77.024	77.672	1.00	0.00	C
ATOM	3009	O	VAL	234	107.491	77.285	76.490	1.00	0.00	O
ATOM	3010	CB	VAL	234	110.287	76.640	77.996	1.00	0.00	C
ATOM	3011	CG1	VAL	234	111.637	77.212	78.478	1.00	0.00	C
ATOM	3012	CG2	VAL	234	110.179	75.177	78.463	1.00	0.00	C
ATOM	3013	H	VAL	234	109.295	77.390	80.522	1.00	0.00	H
ATOM	3014	HA	VAL	234	109.256	78.472	77.736	1.00	0.00	H
ATOM	3015	HB	VAL	234	110.352	76.595	76.889	1.00	0.00	H
ATOM	3016	1HG1	VAL	234	111.830	78.217	78.064	1.00	0.00	H
ATOM	3017	2HG1	VAL	234	111.679	77.294	79.581	1.00	0.00	H
ATOM	3018	3HG1	VAL	234	112.485	76.569	78.180	1.00	0.00	H
ATOM	3019	2HG2	VAL	234	109.275	74.691	78.054	1.00	0.00	H
ATOM	3020	3HG2	VAL	234	111.032	74.567	78.108	1.00	0.00	H
ATOM	3021	1HG2	VAL	234	110.144	75.080	79.563	1.00	0.00	H
ATOM	3022	N	TRP	235	106.805	76.370	78.426	0.00	0.00	N
ATOM	3023	CA	TRP	235	105.377	76.190	78.008	0.00	0.00	C
ATOM	3024	C	TRP	235	104.631	77.524	77.617	0.00	0.00	C
ATOM	3025	O	TRP	235	104.044	77.605	76.537	0.00	0.00	O
ATOM	3026	CB	TRP	235	104.678	75.370	79.134	0.00	0.00	C
ATOM	3027	CG	TRP	235	103.237	74.907	78.840	0.00	0.00	C
ATOM	3028	CD1	TRP	235	102.087	75.732	78.847	0.00	0.00	C
ATOM	3029	NE1	TRP	235	100.919	75.016	78.528	0.00	0.00	N
ATOM	3030	CE2	TRP	235	101.363	73.731	78.340	0.00	0.00	C
ATOM	3031	CD2	TRP	235	102.767	73.836	78.514	0.00	0.00	C
ATOM	3032	CE3	TRP	235	103.127	72.638	78.334	0.00	0.00	C
ATOM	3033	CZ3	TRP	235	104.435	72.235	78.121	0.00	0.00	C
ATOM	3034	CH2	TRP	235	105.388	73.221	78.121	0.00	0.00	C
ATOM	3035	CZ2	TRP	235	105.035	74.533	78.334	0.00	0.00	C

ATOM	3044	HH2	TRP	235	100.726	70.451	77.675	0.00	0.00	H
ATOM	3045	HZ2	TRP	235	99.552	72.617	77.872	0.00	0.00	H
ATOM	3046	N	SER	236	104.693	78.574	78.457	1.00	0.00	N
ATOM	3047	CA	SER	236	104.260	79.951	78.074	1.00	0.00	C
ATOM	3048	C	SER	236	105.007	80.630	76.859	1.00	0.00	C
ATOM	3049	O	SER	236	104.369	81.372	76.112	1.00	0.00	O
ATOM	3050	CB	SER	236	104.309	80.831	79.347	1.00	0.00	C
ATOM	3051	OG	SER	236	103.493	80.340	80.418	1.00	0.00	O
ATOM	3052	H	SER	236	105.222	78.388	79.317	1.00	0.00	H
ATOM	3053	HA	SER	236	103.196	79.893	77.768	1.00	0.00	H
ATOM	3054	1HB	SER	236	105.351	80.918	79.709	1.00	0.00	H
ATOM	3055	2HB	SER	236	103.998	81.867	79.110	1.00	0.00	H
ATOM	3056	HG	SER	236	102.778	79.795	80.055	1.00	0.00	H
ATOM	3057	N	ILE	237	106.309	80.357	76.616	1.00	0.00	N
ATOM	3058	CA	ILE	237	107.003	80.705	75.321	1.00	0.00	C
ATOM	3059	C	ILE	237	106.456	79.903	74.072	1.00	0.00	C
ATOM	3060	O	ILE	237	106.248	80.500	73.014	1.00	0.00	O
ATOM	3061	CB	ILE	237	108.578	80.663	75.438	1.00	0.00	C
ATOM	3062	CG1	ILE	237	109.157	81.505	76.618	1.00	0.00	C
ATOM	3063	CG2	ILE	237	109.275	81.142	74.129	1.00	0.00	C
ATOM	3064	CD1	ILE	237	110.646	81.287	76.949	1.00	0.00	C
ATOM	3065	H	ILE	237	106.740	79.761	77.333	1.00	0.00	H
ATOM	3066	HA	ILE	237	106.758	81.763	75.117	1.00	0.00	H
ATOM	3067	HB	ILE	237	108.860	79.603	75.604	1.00	0.00	H
ATOM	3068	1HG1	ILE	237	108.966	82.579	76.437	1.00	0.00	H
ATOM	3069	2HG1	ILE	237	108.591	81.285	77.540	1.00	0.00	H
ATOM	3070	2HG2	ILE	237	108.960	80.560	73.244	1.00	0.00	H
ATOM	3071	3HG2	ILE	237	109.062	82.205	73.906	1.00	0.00	H
ATOM	3072	1HG2	ILE	237	110.374	81.034	74.173	1.00	0.00	H
ATOM	3073	2HD1	ILE	237	110.884	80.218	77.100	1.00	0.00	H
ATOM	3074	3HD1	ILE	237	111.312	81.668	76.152	1.00	0.00	H
ATOM	3075	1HD1	ILE	237	110.933	81.818	77.875	1.00	0.00	H
ATOM	3076	N	GLY	238	106.200	78.583	74.167	0.00	0.00	N
ATOM	3077	CA	GLY	238	105.387	77.841	73.149	0.00	0.00	C
ATOM	3078	C	GLY	238	103.976	78.385	72.795	0.00	0.00	C
ATOM	3079	O	GLY	238	103.633	78.481	71.615	0.00	0.00	O
ATOM	3080	H	GLY	238	106.452	78.180	75.081	0.00	0.00	H
ATOM	3081	1HA	GLY	238	105.261	76.799	73.491	0.00	0.00	H
ATOM	3082	2HA	GLY	238	105.967	77.757	72.212	0.00	0.00	H
ATOM	3083	N	CYS	239	103.189	78.784	73.803	1.00	0.00	N
ATOM	3084	CA	CYS	239	101.955	79.588	73.598	1.00	0.00	C
ATOM	3085	C	CYS	239	102.130	81.037	73.017	1.00	0.00	C
ATOM	3086	O	CYS	239	101.320	81.424	72.177	1.00	0.00	O
ATOM	3087	CB	CYS	239	101.175	79.555	74.929	1.00	0.00	C
ATOM	3088	SG	CYS	239	100.684	77.847	75.353	1.00	0.00	S
ATOM	3089	H	CYS	239	103.559	78.560	74.737	1.00	0.00	H
ATOM	3090	HA	CYS	239	101.333	79.056	72.854	1.00	0.00	H
ATOM	3091	1HB	CYS	239	101.770	79.984	75.756	1.00	0.00	H
ATOM	3092	2HB	CYS	239	100.257	80.168	74.857	1.00	0.00	H
ATOM	3093	HG	CYS	239	99.879	78.149	76.369	1.00	0.00	H
ATOM	3094	N	ILE	240	103.144	81.846	73.401	1.00	0.00	N
ATOM	3095	CA	ILE	240	103.446	83.157	72.720	1.00	0.00	C
ATOM	3096	C	ILE	240	103.857	83.041	71.205	1.00	0.00	C
ATOM	3097	O	ILE	240	103.322	83.776	70.376	1.00	0.00	O
ATOM	3098	CB	ILE	240	104.363	84.074	73.623	1.00	0.00	C
ATOM	3099	CG1	ILE	240	104.030	85.592	73.537	1.00	0.00	C
ATOM	3100	CG2	ILE	240	105.884	83.930	73.375	1.00	0.00	C
ATOM	3101	CD1	ILE	240	102.718	86.012	74.219	1.00	0.00	C
ATOM	3102	H	ILE	240	103.768	81.425	74.103	1.00	0.00	H
ATOM	3103	HA	ILE	240	102.475	83.683	72.661	1.00	0.00	H
ATOM	3104	HB	ILE	240	104.204	83.784	74.683	1.00	0.00	H
ATOM	3105	1HG1	ILE	240	104.839	86.186	74.008	1.00	0.00	H
ATOM	3106	2HG1	ILE	240	104.027	85.921	72.479	1.00	0.00	H
ATOM	3107	2HG2	ILE	240	106.194	82.878	73.307	1.00	0.00	H
ATOM	3108	3HG2	ILE	240	106.204	84.406	72.428	1.00	0.00	H
ATOM	3109	1HG2	ILE	240	106.480	84.382	74.189	1.00	0.00	H
ATOM	3110	2HD1	ILE	240	101.825	85.624	73.696	1.00	0.00	H
ATOM	3111	3HD1	ILE	240	102.667	85.675	75.270	1.00	0.00	H
ATOM	3112	1HD1	ILE	240	102.619	87.114	74.233	1.00	0.00	H
ATOM	3113	N	MET	241	104.735	82.087	70.837	1.00	0.00	N
ATOM	3114	CA	MET	241	104.976	81.681	69.418	1.00	0.00	C
ATOM	3115	C	MET	241	103.699	81.313	68.578	1.00	0.00	C
ATOM	3116	O	MET	241	103.509	81.859	67.490	1.00	0.00	O

ATOM	3117	CB	MET	241	106.015	80.527	69.488	1.00	0.00	C
ATOM	3118	CG	MET	241	106.567	80.031	68.129	1.00	0.00	C
ATOM	3119	SD	MET	241	107.621	78.555	68.239	1.00	0.00	S
ATOM	3120	CE	MET	241	108.499	78.673	69.810	1.00	0.00	C
ATOM	3121	H	MET	241	105.091	81.530	71.626	1.00	0.00	H
ATOM	3122	HA	MET	241	105.453	82.535	68.899	1.00	0.00	H
ATOM	3123	1HB	MET	241	106.874	80.850	70.110	1.00	0.00	H
ATOM	3124	2HB	MET	241	105.577	79.664	70.029	1.00	0.00	H
ATOM	3125	1HG	MET	241	105.735	79.767	67.450	1.00	0.00	H
ATOM	3126	2HG	MET	241	107.116	80.834	67.606	1.00	0.00	H
ATOM	3127	1HE	MET	241	109.111	79.588	69.866	1.00	0.00	H
ATOM	3128	3HE	MET	241	107.793	78.671	70.659	1.00	0.00	H
ATOM	3129	2HE	MET	241	109.169	77.807	69.936	1.00	0.00	H
ATOM	3130	N	TYR	242	102.832	80.420	69.086	0.00	0.00	N
ATOM	3131	CA	TYR	242	101.524	80.095	68.447	0.00	0.00	C
ATOM	3132	C	TYR	242	100.518	81.301	68.359	0.00	0.00	C
ATOM	3133	O	TYR	242	100.074	81.616	67.254	0.00	0.00	O
ATOM	3134	CB	TYR	242	100.977	78.843	69.192	0.00	0.00	C
ATOM	3135	CG	TYR	242	99.848	78.067	68.487	0.00	0.00	C
ATOM	3136	CD1	TYR	242	98.549	78.587	68.430	0.00	0.00	C
ATOM	3137	CE1	TYR	242	97.505	77.821	67.920	0.00	0.00	C
ATOM	3138	CZ	TYR	242	97.747	76.525	67.476	0.00	0.00	C
ATOM	3139	OH	TYR	242	96.709	75.742	67.055	0.00	0.00	O
ATOM	3140	CE2	TYR	242	99.037	76.005	67.506	0.00	0.00	C
ATOM	3141	CD2	TYR	242	100.086	76.773	68.008	0.00	0.00	C
ATOM	3142	H	TYR	242	103.082	79.937	69.961	1.00	0.00	H
ATOM	3143	HA	TYR	242	101.733	79.791	67.401	0.00	0.00	H
ATOM	3144	1HB	TYR	242	100.640	79.136	70.204	0.00	0.00	H
ATOM	3145	2HB	TYR	242	101.809	78.139	69.399	0.00	0.00	H
ATOM	3146	HD1	TYR	242	98.325	79.574	68.813	0.00	0.00	H
ATOM	3147	HE1	TYR	242	96.504	78.227	67.911	0.00	0.00	H
ATOM	3148	HH	TYR	242	95.880	76.166	67.285	0.00	0.00	H
ATOM	3149	HE2	TYR	242	99.213	74.992	67.173	0.00	0.00	H
ATOM	3150	HD2	TYR	242	101.076	76.342	68.058	0.00	0.00	H
ATOM	3151	N	THR	243	100.184	81.981	69.478	1.00	0.00	N
ATOM	3152	CA	THR	243	99.285	83.185	69.481	1.00	0.00	C
ATOM	3153	C	THR	243	99.713	84.342	68.514	1.00	0.00	C
ATOM	3154	O	THR	243	98.888	84.807	67.726	1.00	0.00	O
ATOM	3155	CB	THR	243	99.090	83.743	70.932	1.00	0.00	C
ATOM	3156	OG1	THR	243	98.832	82.718	71.884	1.00	0.00	O
ATOM	3157	CG2	THR	243	97.910	84.721	71.059	1.00	0.00	C
ATOM	3158	H	THR	243	100.655	81.660	70.333	1.00	0.00	H
ATOM	3159	HA	THR	243	98.293	82.839	69.129	1.00	0.00	H
ATOM	3160	HB	THR	243	100.024	84.260	71.238	1.00	0.00	H
ATOM	3161	HG1	THR	243	99.139	83.061	72.734	1.00	0.00	H
ATOM	3162	1HG2	THR	243	97.704	85.005	72.105	1.00	0.00	H
ATOM	3163	2HG2	THR	243	98.085	85.655	70.491	1.00	0.00	H
ATOM	3164	3HG2	THR	243	96.979	84.281	70.658	1.00	0.00	H
ATOM	3165	N	LEU	244	100.985	84.781	68.545	1.00	0.00	N
ATOM	3166	CA	LEU	244	101.545	85.737	67.545	1.00	0.00	C
ATOM	3167	C	LEU	244	101.478	85.258	66.049	1.00	0.00	C
ATOM	3168	O	LEU	244	101.053	86.030	65.189	1.00	0.00	O
ATOM	3169	CB	LEU	244	102.996	86.108	67.971	1.00	0.00	C
ATOM	3170	CG	LEU	244	103.197	86.828	69.336	1.00	0.00	C
ATOM	3171	CD1	LEU	244	104.693	86.857	69.681	1.00	0.00	C
ATOM	3172	CD2	LEU	244	102.634	88.258	69.364	1.00	0.00	C
ATOM	3173	H	LEU	244	101.595	84.257	69.185	1.00	0.00	H
ATOM	3174	HA	LEU	244	100.944	86.664	67.584	1.00	0.00	H
ATOM	3175	1HB	LEU	244	103.333	85.177	67.962	1.00	0.00	H
ATOM	3176	2HB	LEU	244	103.453	86.722	67.179	1.00	0.00	H
ATOM	3177	HG	LEU	244	102.492	88.247	70.157	1.00	0.00	H
ATOM	3178	1HD1	LEU	244	105.105	87.287	70.457	1.00	0.00	H

ATOM	3190	CD1	LEU	245	103.344	82.362	61.820	1.00	0.00	C
ATOM	3191	CD2	LEU	245	103.963	80.340	63.152	1.00	0.00	C
ATOM	3192	H	LEU	245	102.133	83.433	66.548	1.00	0.00	H
ATOM	3193	HA	LEU	245	102.271	84.194	63.697	1.00	0.00	H
ATOM	3194	1HB	LEU	245	103.730	82.513	64.700	1.00	0.00	H
ATOM	3195	2HB	LEU	245	102.371	81.475	65.084	1.00	0.00	H
ATOM	3196	HG	LEU	245	101.953	80.980	62.714	1.00	0.00	H
ATOM	3197	2HD1	LEU	245	102.592	83.146	61.614	1.00	0.00	H
ATOM	3198	3HD1	LEU	245	104.301	82.881	62.016	1.00	0.00	H
ATOM	3199	1HD1	LEU	245	103.446	81.789	60.880	1.00	0.00	H
ATOM	3200	2HD2	LEU	245	104.967	80.740	63.387	1.00	0.00	H
ATOM	3201	3HD2	LEU	245	103.690	79.650	63.972	1.00	0.00	H
ATOM	3202	1HD2	LEU	245	104.055	79.729	62.234	1.00	0.00	H
ATOM	3203	N	VAL	246	99.420	82.532	64.412	1.00	0.00	N
ATOM	3204	CA	VAL	246	98.018	82.373	63.887	1.00	0.00	C
ATOM	3205	C	VAL	246	97.012	83.542	64.197	1.00	0.00	C
ATOM	3206	O	VAL	246	96.113	83.787	63.387	1.00	0.00	O
ATOM	3207	CB	VAL	246	97.466	80.939	64.220	1.00	0.00	C
ATOM	3208	CG1	VAL	246	97.060	80.705	65.691	1.00	0.00	C
ATOM	3209	CG2	VAL	246	96.256	80.541	63.340	1.00	0.00	C
ATOM	3210	H	VAL	246	99.698	82.253	65.364	1.00	0.00	H
ATOM	3211	HA	VAL	246	98.082	82.391	62.781	1.00	0.00	H
ATOM	3212	HB	VAL	246	98.274	80.217	63.987	1.00	0.00	H
ATOM	3213	1HG1	VAL	246	96.219	81.348	66.008	1.00	0.00	H
ATOM	3214	2HG1	VAL	246	96.751	79.661	65.873	1.00	0.00	H
ATOM	3215	3HG1	VAL	246	97.889	80.912	66.389	1.00	0.00	H
ATOM	3216	2HG2	VAL	246	96.503	80.566	62.265	1.00	0.00	H
ATOM	3217	3HG2	VAL	246	95.894	79.519	63.559	1.00	0.00	H
ATOM	3218	1HG2	VAL	246	95.393	81.219	63.488	1.00	0.00	H
ATOM	3219	N	GLY	247	97.099	84.206	65.360	0.00	0.00	N
ATOM	3220	CA	GLY	247	96.020	85.100	65.871	0.00	0.00	C
ATOM	3221	C	GLY	247	95.492	84.695	67.263	0.00	0.00	C
ATOM	3222	O	GLY	247	95.697	85.401	68.254	0.00	0.00	O
ATOM	3223	H	GLY	247	97.934	83.977	65.917	0.00	0.00	H
ATOM	3224	1HA	GLY	247	95.163	85.180	65.173	0.00	0.00	H
ATOM	3225	2HA	GLY	247	96.403	86.132	65.927	0.00	0.00	H
ATOM	3226	N	LYS	248	94.784	83.561	67.320	1.00	0.00	N
ATOM	3227	CA	LYS	248	94.201	83.016	68.579	1.00	0.00	C
ATOM	3228	C	LYS	248	95.191	82.099	69.402	1.00	0.00	C
ATOM	3229	O	LYS	248	95.994	81.382	68.791	1.00	0.00	O
ATOM	3230	CB	LYS	248	92.912	82.231	68.204	1.00	0.00	C
ATOM	3231	CG	LYS	248	91.705	83.103	67.777	1.00	0.00	C
ATOM	3232	CD	LYS	248	90.498	82.257	67.331	1.00	0.00	C
ATOM	3233	CE	LYS	248	89.278	83.127	66.999	1.00	0.00	C
ATOM	3234	NZ	LYS	248	88.159	82.262	66.577	1.00	0.00	N
ATOM	3235	1HZ	LYS	248	87.339	82.845	66.354	1.00	0.00	H
ATOM	3236	2HZ	LYS	248	88.436	81.725	65.743	1.00	0.00	H
ATOM	3237	3HZ	LYS	248	87.920	81.612	67.339	1.00	0.00	H
ATOM	3238	H	LYS	248	94.798	83.034	66.443	1.00	0.00	H
ATOM	3239	HA	LYS	248	93.904	83.868	69.219	1.00	0.00	H
ATOM	3240	1HB	LYS	248	93.145	81.487	67.415	1.00	0.00	H
ATOM	3241	2HB	LYS	248	92.596	81.613	69.067	1.00	0.00	H
ATOM	3242	1HG	LYS	248	91.419	83.774	68.610	1.00	0.00	H
ATOM	3243	2HG	LYS	248	92.002	83.776	66.948	1.00	0.00	H
ATOM	3244	1HD	LYS	248	90.780	81.656	66.443	1.00	0.00	H
ATOM	3245	2HD	LYS	248	90.239	81.516	68.112	1.00	0.00	H
ATOM	3246	1HE	LYS	248	88.979	83.741	67.873	1.00	0.00	H
ATOM	3247	2HE	LYS	248	89.524	83.843	66.188	1.00	0.00	H
ATOM	3248	N	PRO	249	95.154	82.039	70.771	0.00	0.00	N
ATOM	3249	CA	PRO	249	96.020	81.112	71.555	0.00	0.00	C
ATOM	3250	CD	PRO	249	94.324	82.923	71.609	0.00	0.00	C
ATOM	3251	C	PRO	249	95.717	79.571	71.421	0.00	0.00	C
ATOM	3252	O	PRO	249	94.594	79.206	71.051	0.00	0.00	O
ATOM	3253	CB	PRO	249	95.856	81.670	72.986	0.00	0.00	C
ATOM	3254	CG	PRO	249	94.475	82.324	73.005	0.00	0.00	C
ATOM	3255	HA	PRO	249	97.059	81.260	71.214	0.00	0.00	H
ATOM	3256	1HD	PRO	249	93.266	82.947	71.289	0.00	0.00	H
ATOM	3257	2HD	PRO	249	94.709	83.962	71.575	0.00	0.00	H
ATOM	3258	1HB	PRO	249	96.635	82.431	73.179	0.00	0.00	H
ATOM	3259	2HB	PRO	249	95.969	80.898	73.772	0.00	0.00	H
ATOM	3260	1HG	PRO	249	94.358	83.079	73.801	0.00	0.00	H
ATOM	3261	2HG	PRO	249	93.697	81.554	73.164	0.00	0.00	H
ATOM	3262	N	PRO	250	96.669	78.630	71.710	0.00	0.00	N

ATOM	3263	CA	PRO	250	96.501	77.190	71.345	0.00	0.00	C
ATOM	3264	CD	PRO	250	98.027	78.957	72.199	0.00	0.00	C
ATOM	3265	C	PRO	250	95.405	76.338	72.063	0.00	0.00	C
ATOM	3266	O	PRO	250	94.769	75.510	71.408	0.00	0.00	O
ATOM	3267	CB	PRO	250	97.937	76.661	71.500	0.00	0.00	C
ATOM	3268	CG	PRO	250	98.615	77.582	72.511	0.00	0.00	C
ATOM	3269	HA	PRO	250	96.236	77.132	70.273	0.00	0.00	H
ATOM	3270	1HD	PRO	250	98.022	79.609	73.093	0.00	0.00	H
ATOM	3271	2HD	PRO	250	98.612	79.473	71.412	0.00	0.00	H
ATOM	3272	1HB	PRO	250	98.465	76.713	70.531	0.00	0.00	H
ATOM	3273	2HB	PRO	250	97.983	75.602	71.782	0.00	0.00	H
ATOM	3274	1HG	PRO	250	99.717	77.552	72.427	0.00	0.00	H
ATOM	3275	2HG	PRO	250	98.359	77.276	73.544	0.00	0.00	H
ATOM	3276	N	PHE	251	95.171	76.536	73.369	0.00	0.00	N
ATOM	3277	CA	PHE	251	93.963	75.999	74.056	0.00	0.00	C
ATOM	3278	C	PHE	251	93.134	77.170	74.676	0.00	0.00	C
ATOM	3279	O	PHE	251	93.535	77.784	75.669	0.00	0.00	O
ATOM	3280	CB	PHE	251	94.359	74.924	75.110	0.00	0.00	C
ATOM	3281	CG	PHE	251	94.855	73.539	74.627	0.00	0.00	C
ATOM	3282	CD1	PHE	251	94.370	72.914	73.468	0.00	0.00	C
ATOM	3283	CE1	PHE	251	94.778	71.624	73.136	0.00	0.00	C
ATOM	3284	CZ	PHE	251	95.658	70.940	73.966	0.00	0.00	C
ATOM	3285	CE2	PHE	251	96.139	71.542	75.122	0.00	0.00	C
ATOM	3286	CD2	PHE	251	95.739	72.836	75.452	0.00	0.00	C
ATOM	3287	H	PHE	251	95.711	77.322	73.743	0.00	0.00	H
ATOM	3288	HA	PHE	251	93.295	75.495	73.329	0.00	0.00	H
ATOM	3289	1HB	PHE	251	93.478	74.727	75.750	0.00	0.00	H
ATOM	3290	2HB	PHE	251	95.092	75.375	75.806	0.00	0.00	H
ATOM	3291	HD1	PHE	251	93.671	73.410	72.814	0.00	0.00	H
ATOM	3292	HE1	PHE	251	94.410	71.151	72.236	0.00	0.00	H
ATOM	3293	HZ	PHE	251	95.972	69.941	73.707	0.00	0.00	H
ATOM	3294	HE2	PHE	251	96.825	71.005	75.763	0.00	0.00	H
ATOM	3295	HD2	PHE	251	96.115	73.283	76.358	0.00	0.00	H
ATOM	3296	N	GLU	252	91.963	77.457	74.083	1.00	0.00	N
ATOM	3297	CA	GLU	252	90.978	78.433	74.629	1.00	0.00	C
ATOM	3298	C	GLU	252	89.511	77.887	74.512	1.00	0.00	C
ATOM	3299	O	GLU	252	88.774	78.205	73.573	1.00	0.00	O
ATOM	3300	CB	GLU	252	91.191	79.843	74.006	1.00	0.00	C
ATOM	3301	CG	GLU	252	91.120	79.990	72.457	1.00	0.00	C
ATOM	3302	CD	GLU	252	90.880	81.410	71.943	1.00	0.00	C
ATOM	3303	OE1	GLU	252	91.116	82.435	72.575	1.00	0.00	O
ATOM	3304	OE2	GLU	252	90.369	81.410	70.683	1.00	0.00	O
ATOM	3305	H	GLU	252	91.798	76.958	73.202	1.00	0.00	H
ATOM	3306	HA	GLU	252	91.157	78.567	75.716	1.00	0.00	H
ATOM	3307	1HB	GLU	252	90.450	80.523	74.472	1.00	0.00	H
ATOM	3308	2HB	GLU	252	92.170	80.226	74.346	1.00	0.00	H
ATOM	3309	1HG	GLU	252	92.052	79.611	71.998	1.00	0.00	H
ATOM	3310	2HG	GLU	252	90.319	79.351	72.044	1.00	0.00	H
ATOM	3311	N	THR	253	89.078	77.064	75.479	1.00	0.00	N
ATOM	3312	CA	THR	253	87.671	76.555	75.551	1.00	0.00	C
ATOM	3313	C	THR	253	86.821	77.456	76.525	1.00	0.00	C
ATOM	3314	O	THR	253	87.348	78.092	77.442	1.00	0.00	O
ATOM	3315	CB	THR	253	87.705	75.025	75.879	1.00	0.00	C
ATOM	3316	OG1	THR	253	88.536	74.338	74.942	1.00	0.00	O
ATOM	3317	CG2	THR	253	86.347	74.314	75.773	1.00	0.00	C
ATOM	3318	H	THR	253	89.751	76.885	76.233	1.00	0.00	H
ATOM	3319	HA	THR	253	87.207	76.633	74.548	1.00	0.00	H
ATOM	3320	HB	THR	253	88.122	74.883	76.897	1.00	0.00	H
ATOM	3321	HG1	THR	253	88.566	73.390	75.277	1.00	0.00	H
ATOM	3322	1HG2	THR	253	86.343	73.225	76.002	1.00	0.00	H
ATOM	3323	2HG2	THR	253	85.601	74.772	75.139	1.00	0.00	H
ATOM	3324	3HG2	THR	253	86.401	74.238	76.778	1.00	0.00	H
ATOM	3325	[illegible]								

ATOM	3336	N	CYS	255	85.100	78.129	79.298	1.00	0.00	N
ATOM	3337	CA	CYS	255	85.274	78.483	80.735	1.00	0.00	C
ATOM	3338	C	CYS	255	86.653	77.980	81.291	1.00	0.00	C
ATOM	3339	O	CYS	255	87.287	77.081	80.727	1.00	0.00	O
ATOM	3340	CB	CYS	255	84.059	77.949	81.532	1.00	0.00	C
ATOM	3341	SG	CYS	255	83.991	76.125	81.530	1.00	0.00	S
ATOM	3342	H	CYS	255	85.801	77.541	78.829	1.00	0.00	H
ATOM	3343	HA	CYS	255	85.285	79.588	80.834	1.00	0.00	H
ATOM	3344	1HB	CYS	255	84.098	78.298	82.579	1.00	0.00	H
ATOM	3345	2HB	CYS	255	83.111	78.350	81.122	1.00	0.00	H
ATOM	3346	HG	CYS	255	83.576	75.982	80.275	1.00	0.00	H
ATOM	3347	N	LEU	256	87.110	78.539	82.429	1.00	0.00	N
ATOM	3348	CA	LEU	256	88.437	78.204	83.043	1.00	0.00	C
ATOM	3349	C	LEU	256	88.717	76.678	83.289	1.00	0.00	C
ATOM	3350	O	LEU	256	89.732	76.166	82.819	1.00	0.00	O
ATOM	3351	CB	LEU	256	88.641	79.036	84.347	1.00	0.00	C
ATOM	3352	CG	LEU	256	88.951	80.551	84.214	1.00	0.00	C
ATOM	3353	CD1	LEU	256	87.723	81.413	83.867	1.00	0.00	C
ATOM	3354	CD2	LEU	256	89.546	81.077	85.533	1.00	0.00	C
ATOM	3355	H	LEU	256	86.525	79.294	82.798	1.00	0.00	H
ATOM	3356	HA	LEU	256	89.222	78.522	82.328	1.00	0.00	H
ATOM	3357	1HB	LEU	256	87.794	78.878	85.043	1.00	0.00	H
ATOM	3358	2HB	LEU	256	89.502	78.580	84.880	1.00	0.00	H
ATOM	3359	HG	LEU	256	89.710	80.687	83.419	1.00	0.00	H
ATOM	3360	2HD1	LEU	256	87.335	81.198	82.857	1.00	0.00	H
ATOM	3361	3HD1	LEU	256	86.893	81.266	84.584	1.00	0.00	H
ATOM	3362	1HD1	LEU	256	87.965	82.492	83.872	1.00	0.00	H
ATOM	3363	2HD2	LEU	256	88.839	80.978	86.380	1.00	0.00	H
ATOM	3364	3HD2	LEU	256	90.465	80.530	85.818	1.00	0.00	H
ATOM	3365	1HD2	LEU	256	89.825	82.144	85.467	1.00	0.00	H
ATOM	3366	N	LYS	257	87.800	75.951	83.953	1.00	0.00	N
ATOM	3367	CA	LYS	257	87.873	74.462	84.089	1.00	0.00	C
ATOM	3368	C	LYS	257	87.861	73.614	82.764	1.00	0.00	C
ATOM	3369	O	LYS	257	88.490	72.555	82.727	1.00	0.00	O
ATOM	3370	CB	LYS	257	86.754	74.003	85.066	1.00	0.00	C
ATOM	3371	CG	LYS	257	86.922	74.460	86.537	1.00	0.00	C
ATOM	3372	CD	LYS	257	85.765	73.981	87.434	1.00	0.00	C
ATOM	3373	CE	LYS	257	85.926	74.466	88.881	1.00	0.00	C
ATOM	3374	NZ	LYS	257	84.781	73.996	89.685	1.00	0.00	N
ATOM	3375	1HZ	LYS	257	84.887	74.321	90.657	1.00	0.00	H
ATOM	3376	2HZ	LYS	257	83.906	74.372	89.292	1.00	0.00	H
ATOM	3377	3HZ	LYS	257	84.749	72.967	89.670	1.00	0.00	H
ATOM	3378	H	LYS	257	86.991	76.492	84.272	1.00	0.00	H
ATOM	3379	HA	LYS	257	88.840	74.217	84.568	1.00	0.00	H
ATOM	3380	1HB	LYS	257	85.766	74.319	84.678	1.00	0.00	H
ATOM	3381	2HB	LYS	257	86.711	72.897	85.064	1.00	0.00	H
ATOM	3382	1HG	LYS	257	87.885	74.087	86.937	1.00	0.00	H
ATOM	3383	2HG	LYS	257	86.992	75.564	86.588	1.00	0.00	H
ATOM	3384	1HD	LYS	257	84.800	74.343	87.025	1.00	0.00	H
ATOM	3385	2HD	LYS	257	85.706	72.875	87.407	1.00	0.00	H
ATOM	3386	1HE	LYS	257	86.877	74.097	89.316	1.00	0.00	H
ATOM	3387	2HE	LYS	257	85.978	75.573	88.918	1.00	0.00	H
ATOM	3388	N	GLU	258	87.189	74.064	81.686	1.00	0.00	N
ATOM	3389	CA	GLU	258	87.332	73.448	80.332	1.00	0.00	C
ATOM	3390	C	GLU	258	88.705	73.711	79.619	1.00	0.00	C
ATOM	3391	O	GLU	258	89.293	72.754	79.114	1.00	0.00	O
ATOM	3392	CB	GLU	258	86.118	73.847	79.451	1.00	0.00	C
ATOM	3393	CG	GLU	258	84.750	73.213	79.823	1.00	0.00	C
ATOM	3394	CD	GLU	258	84.645	71.709	79.571	1.00	0.00	C
ATOM	3395	OE1	GLU	258	84.362	71.217	78.485	1.00	0.00	O
ATOM	3396	OE2	GLU	258	84.899	70.977	80.687	1.00	0.00	O
ATOM	3397	H	GLU	258	86.861	75.028	81.801	1.00	0.00	H
ATOM	3398	HA	GLU	258	87.289	72.346	80.451	1.00	0.00	H
ATOM	3399	1HB	GLU	258	86.027	74.951	79.425	1.00	0.00	H
ATOM	3400	2HB	GLU	258	86.339	73.566	78.406	1.00	0.00	H
ATOM	3401	1HG	GLU	258	84.495	73.423	80.877	1.00	0.00	H
ATOM	3402	2HG	GLU	258	83.951	73.695	79.230	1.00	0.00	H
ATOM	3403	N	THR	259	89.256	74.941	79.608	1.00	0.00	N
ATOM	3404	CA	THR	259	90.700	75.186	79.255	1.00	0.00	C
ATOM	3405	C	THR	259	91.743	74.348	80.089	1.00	0.00	C
ATOM	3406	O	THR	259	92.662	73.765	79.509	1.00	0.00	O
ATOM	3407	CB	THR	259	90.988	76.720	79.303	1.00	0.00	C
ATOM	3408	OG1	THR	259	90.192	77.414	78.352	1.00	0.00	O

ATOM	3409	CG2	THR	259	92.425	77.133	78.955	1.00	0.00	C
ATOM	3410	H	THR	259	88.665	75.681	80.011	1.00	0.00	H
ATOM	3411	HA	THR	259	90.841	74.870	78.203	1.00	0.00	H
ATOM	3412	HB	THR	259	90.750	77.097	80.320	1.00	0.00	H
ATOM	3413	HG1	THR	259	90.577	78.292	78.280	1.00	0.00	H
ATOM	3414	1HG2	THR	259	92.562	78.226	79.020	1.00	0.00	H
ATOM	3415	2HG2	THR	259	93.166	76.690	79.646	1.00	0.00	H
ATOM	3416	3HG2	THR	259	92.711	76.823	77.933	1.00	0.00	H
ATOM	3417	N	TYR	260	91.586	74.262	81.423	0.00	0.00	N
ATOM	3418	CA	TYR	260	92.363	73.330	82.294	0.00	0.00	C
ATOM	3419	C	TYR	260	92.279	71.804	81.919	0.00	0.00	C
ATOM	3420	O	TYR	260	93.315	71.139	81.844	0.00	0.00	O
ATOM	3421	CB	TYR	260	91.924	73.570	83.770	0.00	0.00	C
ATOM	3422	CG	TYR	260	92.128	74.943	84.457	0.00	0.00	C
ATOM	3423	CD1	TYR	260	92.987	75.934	83.963	0.00	0.00	C
ATOM	3424	CE1	TYR	260	93.105	77.157	84.618	0.00	0.00	C
ATOM	3425	CZ	TYR	260	92.370	77.402	85.772	0.00	0.00	C
ATOM	3426	OH	TYR	260	92.494	78.601	86.417	0.00	0.00	O
ATOM	3427	CE2	TYR	260	91.523	76.424	86.280	0.00	0.00	C
ATOM	3428	CD2	TYR	260	91.408	75.196	85.631	0.00	0.00	C
ATOM	3429	H	TYR	260	90.890	74.876	81.869	1.00	0.00	H
ATOM	3430	HA	TYR	260	93.435	73.594	82.207	0.00	0.00	H
ATOM	3431	1HB	TYR	260	92.431	72.818	84.399	0.00	0.00	H
ATOM	3432	2HB	TYR	260	90.856	73.289	83.848	0.00	0.00	H
ATOM	3433	HD1	TYR	260	93.564	75.768	83.063	0.00	0.00	H
ATOM	3434	HE1	TYR	260	93.777	77.903	84.231	0.00	0.00	H
ATOM	3435	HH	TYR	260	93.285	79.038	86.094	0.00	0.00	H
ATOM	3436	HE2	TYR	260	90.964	76.616	87.184	0.00	0.00	H
ATOM	3437	HD2	TYR	260	90.752	74.444	86.046	0.00	0.00	H
ATOM	3438	N	LEU	261	91.075	71.265	81.640	1.00	0.00	N
ATOM	3439	CA	LEU	261	90.897	69.932	80.984	1.00	0.00	C
ATOM	3440	C	LEU	261	91.694	69.702	79.646	1.00	0.00	C
ATOM	3441	O	LEU	261	92.322	68.652	79.497	1.00	0.00	O
ATOM	3442	CB	LEU	261	89.358	69.723	80.849	1.00	0.00	C
ATOM	3443	CG	LEU	261	88.856	68.354	80.325	1.00	0.00	C
ATOM	3444	CD1	LEU	261	89.165	67.203	81.298	1.00	0.00	C
ATOM	3445	CD2	LEU	261	87.340	68.412	80.075	1.00	0.00	C
ATOM	3446	H	LEU	261	90.292	71.922	81.746	1.00	0.00	H
ATOM	3447	HA	LEU	261	91.277	69.171	81.692	1.00	0.00	H
ATOM	3448	1HB	LEU	261	88.869	69.924	81.824	1.00	0.00	H
ATOM	3449	2HB	LEU	261	88.967	70.510	80.178	1.00	0.00	H
ATOM	3450	HG	LEU	261	89.350	68.138	79.355	1.00	0.00	H
ATOM	3451	2HD1	LEU	261	90.254	67.069	81.437	1.00	0.00	H
ATOM	3452	3HD1	LEU	261	88.721	67.367	82.298	1.00	0.00	H
ATOM	3453	1HD1	LEU	261	88.781	66.236	80.922	1.00	0.00	H
ATOM	3454	2HD2	LEU	261	86.774	68.623	81.001	1.00	0.00	H
ATOM	3455	3HD2	LEU	261	87.082	69.198	79.340	1.00	0.00	H
ATOM	3456	1HD2	LEU	261	86.959	67.459	79.664	1.00	0.00	H
ATOM	3457	N	ARG	262	91.731	70.679	78.720	1.00	0.00	N
ATOM	3458	CA	ARG	262	92.648	70.647	77.542	1.00	0.00	C
ATOM	3459	C	ARG	262	94.188	70.612	77.880	1.00	0.00	C
ATOM	3460	O	ARG	262	94.905	69.763	77.348	1.00	0.00	O
ATOM	3461	CB	ARG	262	92.340	71.831	76.577	1.00	0.00	C
ATOM	3462	CG	ARG	262	90.899	72.128	76.094	1.00	0.00	C
ATOM	3463	CD	ARG	262	90.194	70.966	75.385	1.00	0.00	C
ATOM	3464	NE	ARG	262	88.899	71.458	74.845	1.00	0.00	N
ATOM	3465	CZ	ARG	262	88.061	70.748	74.099	1.00	0.00	C
ATOM	3466	NH1	ARG	262	88.245	69.501	73.778	1.00	0.00	N
ATOM	3467	NH2	ARG	262	87.005	71.227	73.662	1.00	0.00	N
ATOM	3468	HE	ARG	262	88.631	72.428	75.067	1.00	0.00	H
ATOM	3469	H	ARG	262	91.153	71.197	78.952	1.00	0.00	H

ATOM	3482	CA	ILE	263	96.162	71.638	79.087	0.00	0.00	C
ATOM	3483	C	ILE	263	96.852	70.322	79.595	0.00	0.00	C
ATOM	3484	O	ILE	263	97.919	69.961	79.089	0.00	0.00	O
ATOM	3485	CB	ILE	263	96.358	72.915	79.998	0.00	0.00	C
ATOM	3486	CG2	ILE	263	97.713	72.981	80.760	0.00	0.00	C
ATOM	3487	CG1	ILE	263	96.180	74.229	79.176	0.00	0.00	C
ATOM	3488	CD1	ILE	263	96.033	75.524	79.988	0.00	0.00	C
ATOM	3489	H	ILE	263	93.987	72.147	79.138	0.00	0.00	H
ATOM	3490	HA	ILE	263	96.703	71.848	78.143	0.00	0.00	H
ATOM	3491	HB	ILE	263	95.570	72.886	80.779	0.00	0.00	H
ATOM	3492	1HG2	ILE	263	97.758	73.841	81.453	0.00	0.00	H
ATOM	3493	2HG2	ILE	263	97.888	72.090	81.391	0.00	0.00	H
ATOM	3494	3HG2	ILE	263	98.576	73.073	80.078	0.00	0.00	H
ATOM	3495	1HG1	ILE	263	95.276	74.150	78.541	0.00	0.00	H
ATOM	3496	2HG1	ILE	263	97.018	74.342	78.460	0.00	0.00	H
ATOM	3497	1HD1	ILE	263	95.825	76.385	79.327	0.00	0.00	H
ATOM	3498	2HD1	ILE	263	95.201	75.466	80.716	0.00	0.00	H
ATOM	3499	3HD1	ILE	263	96.952	75.777	80.549	0.00	0.00	H
ATOM	3500	N	LYS	264	96.248	69.602	80.554	1.00	0.00	N
ATOM	3501	CA	LYS	264	96.726	68.247	80.970	1.00	0.00	C
ATOM	3502	C	LYS	264	96.706	67.106	79.876	1.00	0.00	C
ATOM	3503	O	LYS	264	97.548	66.207	79.928	1.00	0.00	O
ATOM	3504	CB	LYS	264	95.936	67.915	82.266	1.00	0.00	C
ATOM	3505	CG	LYS	264	96.507	66.746	83.102	1.00	0.00	C
ATOM	3506	CD	LYS	264	95.859	66.668	84.497	1.00	0.00	C
ATOM	3507	CE	LYS	264	96.455	65.540	85.352	1.00	0.00	C
ATOM	3508	NZ	LYS	264	95.990	65.686	86.747	1.00	0.00	N
ATOM	3509	1HZ	LYS	264	96.389	64.930	87.323	1.00	0.00	H
ATOM	3510	2HZ	LYS	264	96.296	66.597	87.118	1.00	0.00	H
ATOM	3511	3HZ	LYS	264	94.962	65.631	86.775	1.00	0.00	H
ATOM	3512	H	LYS	264	95.332	69.978	80.830	1.00	0.00	H
ATOM	3513	HA	LYS	264	97.791	68.352	81.256	1.00	0.00	H
ATOM	3514	1HB	LYS	264	95.915	68.811	82.921	1.00	0.00	H
ATOM	3515	2HB	LYS	264	94.873	67.717	82.021	1.00	0.00	H
ATOM	3516	1HG	LYS	264	96.375	65.790	82.559	1.00	0.00	H
ATOM	3517	2HG	LYS	264	97.603	66.872	83.218	1.00	0.00	H
ATOM	3518	1HD	LYS	264	95.990	67.646	85.005	1.00	0.00	H
ATOM	3519	2HD	LYS	264	94.763	66.533	84.400	1.00	0.00	H
ATOM	3520	1HE	LYS	264	96.164	64.551	84.944	1.00	0.00	H
ATOM	3521	2HE	LYS	264	97.564	65.563	85.324	1.00	0.00	H
ATOM	3522	N	LYS	265	95.801	67.156	78.879	1.00	0.00	N
ATOM	3523	CA	LYS	265	95.810	66.235	77.699	1.00	0.00	C
ATOM	3524	C	LYS	265	96.949	66.440	76.629	1.00	0.00	C
ATOM	3525	O	LYS	265	97.292	65.473	75.946	1.00	0.00	O
ATOM	3526	CB	LYS	265	94.419	66.320	77.003	1.00	0.00	C
ATOM	3527	CG	LYS	265	93.209	65.795	77.809	1.00	0.00	C
ATOM	3528	CD	LYS	265	91.881	66.006	77.056	1.00	0.00	C
ATOM	3529	CE	LYS	265	90.672	65.560	77.889	1.00	0.00	C
ATOM	3530	NZ	LYS	265	89.430	65.791	77.125	1.00	0.00	N
ATOM	3531	1HZ	LYS	265	88.620	65.492	77.686	1.00	0.00	H
ATOM	3532	2HZ	LYS	265	89.343	66.794	76.905	1.00	0.00	H
ATOM	3533	3HZ	LYS	265	89.460	65.250	76.249	1.00	0.00	H
ATOM	3534	H	LYS	265	95.178	67.973	78.921	1.00	0.00	H
ATOM	3535	HA	LYS	265	95.937	65.197	78.066	1.00	0.00	H
ATOM	3536	1HB	LYS	265	94.232	67.367	76.691	1.00	0.00	H
ATOM	3537	2HB	LYS	265	94.456	65.750	76.053	1.00	0.00	H
ATOM	3538	1HG	LYS	265	93.348	64.723	78.049	1.00	0.00	H
ATOM	3539	2HG	LYS	265	93.160	66.311	78.789	1.00	0.00	H
ATOM	3540	1HD	LYS	265	91.772	67.079	76.801	1.00	0.00	H
ATOM	3541	2HD	LYS	265	91.908	65.464	76.090	1.00	0.00	H
ATOM	3542	1HE	LYS	265	90.760	64.492	78.170	1.00	0.00	H
ATOM	3543	2HE	LYS	265	90.640	66.128	78.842	1.00	0.00	H
ATOM	3544	N	ASN	266	97.497	67.659	76.420	1.00	0.00	N
ATOM	3545	CA	ASN	266	98.622	67.927	75.454	1.00	0.00	C
ATOM	3546	C	ASN	266	98.354	67.785	73.900	1.00	0.00	C
ATOM	3547	O	ASN	266	99.262	68.052	73.108	1.00	0.00	O
ATOM	3548	CB	ASN	266	99.918	67.198	75.952	1.00	0.00	C
ATOM	3549	CG	ASN	266	101.331	67.657	75.554	1.00	0.00	C
ATOM	3550	OD1	ASN	266	102.317	67.035	75.926	1.00	0.00	O
ATOM	3551	ND2	ASN	266	101.533	68.726	74.836	1.00	0.00	N
ATOM	3552	H	ASN	266	97.146	68.365	77.079	1.00	0.00	H
ATOM	3553	HA	ASN	266	98.819	69.010	75.570	1.00	0.00	H
ATOM	3554	1HB	ASN	266	99.928	67.201	77.057	1.00	0.00	H

ATOM	3555	2HB	ASN	266	99.845	66.127	75.691	1.00	0.00	H
ATOM	3556	1HD2	ASN	266	102.525	68.892	74.616	1.00	0.00	H
ATOM	3557	2HD2	ASN	266	100.737	68.989	74.248	1.00	0.00	H
ATOM	3558	N	GLU	267	97.150	67.411	73.431	1.00	0.00	N
ATOM	3559	CA	GLU	267	96.876	67.153	71.985	1.00	0.00	C
ATOM	3560	C	GLU	267	96.696	68.462	71.129	1.00	0.00	C
ATOM	3561	O	GLU	267	95.588	68.985	70.971	1.00	0.00	O
ATOM	3562	CB	GLU	267	95.662	66.183	71.946	1.00	0.00	C
ATOM	3563	CG	GLU	267	95.357	65.583	70.549	1.00	0.00	C
ATOM	3564	CD	GLU	267	94.191	64.600	70.541	1.00	0.00	C
ATOM	3565	OE1	GLU	267	94.308	63.397	70.740	1.00	0.00	O
ATOM	3566	OE2	GLU	267	93.002	65.207	70.284	1.00	0.00	O
ATOM	3567	H	GLU	267	96.511	67.122	74.178	1.00	0.00	H
ATOM	3568	HA	GLU	267	97.734	66.589	71.560	1.00	0.00	H
ATOM	3569	1HB	GLU	267	95.833	65.341	72.650	1.00	0.00	H
ATOM	3570	2HB	GLU	267	94.761	66.704	72.329	1.00	0.00	H
ATOM	3571	1HG	GLU	267	95.145	66.387	69.818	1.00	0.00	H
ATOM	3572	2HG	GLU	267	96.246	65.055	70.155	1.00	0.00	H
ATOM	3573	N	TYR	268	97.801	68.977	70.566	1.00	0.00	N
ATOM	3574	CA	TYR	268	97.809	70.263	69.810	1.00	0.00	C
ATOM	3575	C	TYR	268	97.716	70.049	68.260	1.00	0.00	C
ATOM	3576	O	TYR	268	98.681	69.627	67.613	1.00	0.00	O
ATOM	3577	CB	TYR	268	99.087	71.069	70.197	1.00	0.00	C
ATOM	3578	CG	TYR	268	99.105	71.681	71.610	1.00	0.00	C
ATOM	3579	CD1	TYR	268	99.934	71.160	72.610	1.00	0.00	C
ATOM	3580	CD2	TYR	268	98.293	72.781	71.901	1.00	0.00	C
ATOM	3581	CE1	TYR	268	99.936	71.723	73.886	1.00	0.00	C
ATOM	3582	CE2	TYR	268	98.311	73.348	73.172	1.00	0.00	C
ATOM	3583	CZ	TYR	268	99.135	72.824	74.159	1.00	0.00	C
ATOM	3584	OH	TYR	268	99.129	73.384	75.404	1.00	0.00	O
ATOM	3585	H	TYR	268	98.686	68.459	70.662	1.00	0.00	H
ATOM	3586	HA	TYR	268	96.943	70.887	70.118	1.00	0.00	H
ATOM	3587	1HB	TYR	268	99.988	70.447	70.028	1.00	0.00	H
ATOM	3588	2HB	TYR	268	99.218	71.902	69.480	1.00	0.00	H
ATOM	3589	HD1	TYR	268	100.574	70.315	72.401	1.00	0.00	H
ATOM	3590	HD2	TYR	268	97.630	73.189	71.151	1.00	0.00	H
ATOM	3591	HE1	TYR	268	100.564	71.324	74.667	1.00	0.00	H
ATOM	3592	HE2	TYR	268	97.647	74.166	73.408	1.00	0.00	H
ATOM	3593	HH	TYR	268	98.543	74.141	75.387	1.00	0.00	H
ATOM	3594	N	SER	269	96.568	70.395	67.653	1.00	0.00	N
ATOM	3595	CA	SER	269	96.405	70.397	66.171	1.00	0.00	C
ATOM	3596	C	SER	269	96.971	71.702	65.513	1.00	0.00	C
ATOM	3597	O	SER	269	96.390	72.782	65.646	1.00	0.00	O
ATOM	3598	CB	SER	269	94.904	70.187	65.869	1.00	0.00	C
ATOM	3599	OG	SER	269	94.671	70.101	64.462	1.00	0.00	O
ATOM	3600	H	SER	269	95.820	70.687	68.289	1.00	0.00	H
ATOM	3601	HA	SER	269	96.930	69.519	65.741	1.00	0.00	H
ATOM	3602	1HB	SER	269	94.538	69.257	66.349	1.00	0.00	H
ATOM	3603	2HB	SER	269	94.294	71.008	66.298	1.00	0.00	H
ATOM	3604	HG	SER	269	94.931	70.946	64.075	1.00	0.00	H
ATOM	3605	N	ILE	270	98.101	71.600	64.796	1.00	0.00	N
ATOM	3606	CA	ILE	270	98.790	72.785	64.192	1.00	0.00	C
ATOM	3607	C	ILE	270	98.061	73.392	62.921	1.00	0.00	C
ATOM	3608	O	ILE	270	97.670	72.619	62.038	1.00	0.00	O
ATOM	3609	CB	ILE	270	100.313	72.516	63.902	1.00	0.00	C
ATOM	3610	CG1	ILE	270	100.607	71.347	62.913	1.00	0.00	C
ATOM	3611	CG2	ILE	270	101.142	72.357	65.205	1.00	0.00	C
ATOM	3612	CD1	ILE	270	101.972	71.429	62.207	1.00	0.00	C
ATOM	3613	H	ILE	270	98.550	70.680	64.833	1.00	0.00	H
ATOM	3614	HA	ILE	270	98.791	73.563	64.976	1.00	0.00	H
ATOM	3615	HB	ILE	270	100.693	72.441	63.319	1.00	0.00	H
ATOM	3616	1HG1	ILE	270	100.504	70.375	63.127	1.00	0.00	H

ATOM	3628	O	PRO	271	99.637	75.076	60.365	0.00	0.00	O
ATOM	3629	CB	PRO	271	97.285	76.826	61.795	0.00	0.00	C
ATOM	3630	CG	PRO	271	97.187	76.890	63.320	0.00	0.00	C
ATOM	3631	HA	PRO	271	96.457	74.900	61.214	0.00	0.00	H
ATOM	3632	1HD	PRO	271	99.104	76.028	63.948	0.00	0.00	H
ATOM	3633	2HD	PRO	271	97.663	75.374	64.789	0.00	0.00	H
ATOM	3634	1HB	PRO	271	96.401	77.273	61.302	0.00	0.00	H
ATOM	3635	2HB	PRO	271	98.155	77.425	61.460	0.00	0.00	H
ATOM	3636	1HG	PRO	271	96.138	76.747	63.647	0.00	0.00	H
ATOM	3637	2HG	PRO	271	97.527	77.855	63.736	0.00	0.00	H
ATOM	3638	N	LYS	272	97.848	75.012	59.012	1.00	0.00	N
ATOM	3639	CA	LYS	272	98.620	74.638	57.781	1.00	0.00	C
ATOM	3640	C	LYS	272	99.753	75.604	57.258	1.00	0.00	C
ATOM	3641	O	LYS	272	100.562	75.181	56.429	1.00	0.00	O
ATOM	3642	CB	LYS	272	97.590	74.311	56.660	1.00	0.00	C
ATOM	3643	CG	LYS	272	96.728	73.042	56.890	1.00	0.00	C
ATOM	3644	CD	LYS	272	95.734	72.788	55.741	1.00	0.00	C
ATOM	3645	CE	LYS	272	94.875	71.542	55.996	1.00	0.00	C
ATOM	3646	NZ	LYS	272	93.936	71.353	54.873	1.00	0.00	N
ATOM	3647	1HZ	LYS	272	93.359	70.516	55.044	1.00	0.00	H
ATOM	3648	2HZ	LYS	272	93.326	72.179	54.792	1.00	0.00	H
ATOM	3649	3HZ	LYS	272	94.465	71.231	53.998	1.00	0.00	H
ATOM	3650	H	LYS	272	96.826	74.945	59.037	1.00	0.00	H
ATOM	3651	HA	LYS	272	99.166	73.697	58.001	1.00	0.00	H
ATOM	3652	1HB	LYS	272	96.940	75.189	56.482	1.00	0.00	H
ATOM	3653	2HB	LYS	272	98.135	74.172	55.706	1.00	0.00	H
ATOM	3654	1HG	LYS	272	97.390	72.162	57.013	1.00	0.00	H
ATOM	3655	2HG	LYS	272	96.173	73.124	57.844	1.00	0.00	H
ATOM	3656	1HD	LYS	272	95.079	73.673	55.612	1.00	0.00	H
ATOM	3657	2HD	LYS	272	96.288	72.683	54.786	1.00	0.00	H
ATOM	3658	1HE	LYS	272	95.515	70.644	56.117	1.00	0.00	H
ATOM	3659	2HE	LYS	272	94.310	71.646	56.944	1.00	0.00	H
ATOM	3660	N	HIS	273	99.852	76.859	57.732	0.00	0.00	N
ATOM	3661	CA	HIS	273	101.068	77.716	57.532	0.00	0.00	C
ATOM	3662	C	HIS	273	102.303	77.505	58.495	0.00	0.00	C
ATOM	3663	O	HIS	273	103.356	78.106	58.261	0.00	0.00	O
ATOM	3664	CB	HIS	273	100.609	79.199	57.426	0.00	0.00	C
ATOM	3665	CG	HIS	273	100.004	79.854	58.670	0.00	0.00	C
ATOM	3666	ND1	HIS	273	100.759	80.491	59.641	0.00	0.00	N
ATOM	3667	CE1	HIS	273	99.745	80.966	60.435	0.00	0.00	C
ATOM	3668	NE2	HIS	273	98.441	80.711	60.103	0.00	0.00	N
ATOM	3669	CD2	HIS	273	98.631	79.995	58.934	0.00	0.00	C
ATOM	3670	H	HIS	273	99.200	77.027	58.504	0.00	0.00	H
ATOM	3671	HA	HIS	273	101.491	77.482	56.535	0.00	0.00	H
ATOM	3672	1HB	HIS	273	99.904	79.300	56.580	0.00	0.00	H
ATOM	3673	2HB	HIS	273	101.478	79.808	57.111	0.00	0.00	H
ATOM	3674	HE1	HIS	273	99.988	81.567	61.300	0.00	0.00	H
ATOM	3675	HE2	HIS	273	97.590	81.135	60.489	0.00	0.00	H
ATOM	3676	HD2	HIS	273	97.843	79.641	58.283	0.00	0.00	H
ATOM	3677	N	ILE	274	102.221	76.650	59.534	1.00	0.00	N
ATOM	3678	CA	ILE	274	103.380	76.285	60.408	1.00	0.00	C
ATOM	3679	C	ILE	274	104.287	75.247	59.646	1.00	0.00	C
ATOM	3680	O	ILE	274	103.846	74.144	59.306	1.00	0.00	O
ATOM	3681	CB	ILE	274	102.859	75.786	61.818	1.00	0.00	C
ATOM	3682	CG1	ILE	274	102.352	76.893	62.794	1.00	0.00	C
ATOM	3683	CG2	ILE	274	103.914	74.996	62.640	1.00	0.00	C
ATOM	3684	CD1	ILE	274	101.144	77.724	62.340	1.00	0.00	C
ATOM	3685	H	ILE	274	101.319	76.162	59.609	1.00	0.00	H
ATOM	3686	HA	ILE	274	103.981	77.196	60.601	1.00	0.00	H
ATOM	3687	HB	ILE	274	102.021	75.081	61.635	1.00	0.00	H
ATOM	3688	1HG1	ILE	274	102.069	76.430	63.760	1.00	0.00	H
ATOM	3689	2HG1	ILE	274	103.185	77.575	63.045	1.00	0.00	H
ATOM	3690	2HG2	ILE	274	104.283	74.114	62.088	1.00	0.00	H
ATOM	3691	3HG2	ILE	274	104.802	75.606	62.892	1.00	0.00	H
ATOM	3692	1HG2	ILE	274	103.506	74.600	63.590	1.00	0.00	H
ATOM	3693	2HD1	ILE	274	101.395	78.386	61.491	1.00	0.00	H
ATOM	3694	3HD1	ILE	274	100.312	77.074	62.015	1.00	0.00	H
ATOM	3695	1HD1	ILE	274	100.765	78.375	63.149	1.00	0.00	H
ATOM	3696	N	ASN	275	105.570	75.583	59.420	1.00	0.00	N
ATOM	3697	CA	ASN	275	106.556	74.631	58.827	1.00	0.00	C
ATOM	3698	C	ASN	275	107.024	73.470	59.801	1.00	0.00	C
ATOM	3699	O	ASN	275	106.988	73.680	61.018	1.00	0.00	O
ATOM	3700	CB	ASN	275	107.707	75.475	58.199	1.00	0.00	C

ATOM	3701	CG	ASN	275	108.908	75.847	59.075	1.00	0.00	C
ATOM	3702	OD1	ASN	275	109.770	75.027	59.362	1.00	0.00	O
ATOM	3703	ND2	ASN	275	109.051	77.070	59.501	1.00	0.00	N
ATOM	3704	H	ASN	275	105.796	76.553	59.657	1.00	0.00	H
ATOM	3705	HA	ASN	275	106.038	74.137	57.980	1.00	0.00	H
ATOM	3706	1HB	ASN	275	108.130	74.902	57.357	1.00	0.00	H
ATOM	3707	2HB	ASN	275	107.304	76.377	57.702	1.00	0.00	H
ATOM	3708	1HD2	ASN	275	109.868	77.196	60.104	1.00	0.00	H
ATOM	3709	2HD2	ASN	275	108.261	77.716	59.370	1.00	0.00	H
ATOM	3710	N	PRO	276	107.529	72.281	59.351	1.00	0.00	N
ATOM	3711	CA	PRO	276	108.012	71.204	60.272	1.00	0.00	C
ATOM	3712	C	PRO	276	109.169	71.505	61.293	1.00	0.00	C
ATOM	3713	O	PRO	276	109.175	70.916	62.375	1.00	0.00	O
ATOM	3714	CB	PRO	276	108.317	70.048	59.295	1.00	0.00	C
ATOM	3715	CG	PRO	276	108.521	70.705	57.929	1.00	0.00	C
ATOM	3716	CD	PRO	276	107.552	71.883	57.930	1.00	0.00	C
ATOM	3717	HA	PRO	276	107.154	70.888	60.894	1.00	0.00	H
ATOM	3718	1HB	PRO	276	109.183	69.429	59.600	1.00	0.00	H
ATOM	3719	2HB	PRO	276	107.450	69.360	59.253	1.00	0.00	H
ATOM	3720	1HG	PRO	276	109.564	71.066	57.829	1.00	0.00	H
ATOM	3721	2HG	PRO	276	108.334	70.011	57.088	1.00	0.00	H
ATOM	3722	1HD	PRO	276	107.894	72.676	57.242	1.00	0.00	H
ATOM	3723	2HD	PRO	276	106.538	71.571	57.604	1.00	0.00	H
ATOM	3724	N	VAL	277	110.109	72.418	60.991	1.00	0.00	N
ATOM	3725	CA	VAL	277	111.112	72.927	61.992	1.00	0.00	C
ATOM	3726	C	VAL	277	110.471	73.844	63.108	1.00	0.00	C
ATOM	3727	O	VAL	277	110.775	73.669	64.292	1.00	0.00	O
ATOM	3728	CB	VAL	277	112.343	73.601	61.275	1.00	0.00	C
ATOM	3729	CG1	VAL	277	113.500	73.923	62.250	1.00	0.00	C
ATOM	3730	CG2	VAL	277	112.986	72.778	60.130	1.00	0.00	C
ATOM	3731	H	VAL	277	109.923	72.910	60.110	1.00	0.00	H
ATOM	3732	HA	VAL	277	111.515	72.046	62.533	1.00	0.00	H
ATOM	3733	HB	VAL	277	111.989	74.556	60.836	1.00	0.00	H
ATOM	3734	1HG1	VAL	277	113.946	73.012	62.689	1.00	0.00	H
ATOM	3735	2HG1	VAL	277	114.317	74.489	61.763	1.00	0.00	H
ATOM	3736	3HG1	VAL	277	113.158	74.543	63.096	1.00	0.00	H
ATOM	3737	2HG2	VAL	277	112.267	72.588	59.312	1.00	0.00	H
ATOM	3738	3HG2	VAL	277	113.844	73.303	59.667	1.00	0.00	H
ATOM	3739	1HG2	VAL	277	113.347	71.793	60.477	1.00	0.00	H
ATOM	3740	N	ALA	278	109.573	74.787	62.751	1.00	0.00	N
ATOM	3741	CA	ALA	278	108.679	75.464	63.733	1.00	0.00	C
ATOM	3742	C	ALA	278	107.712	74.540	64.557	1.00	0.00	C
ATOM	3743	O	ALA	278	107.630	74.703	65.775	1.00	0.00	O
ATOM	3744	CB	ALA	278	107.921	76.556	62.955	1.00	0.00	C
ATOM	3745	H	ALA	278	109.333	74.738	61.754	1.00	0.00	H
ATOM	3746	HA	ALA	278	109.320	75.978	64.478	1.00	0.00	H
ATOM	3747	2HB	ALA	278	108.606	77.275	62.472	1.00	0.00	H
ATOM	3748	3HB	ALA	278	107.273	76.132	62.163	1.00	0.00	H
ATOM	3749	1HB	ALA	278	107.267	77.145	63.624	1.00	0.00	H
ATOM	3750	N	ALA	279	107.026	73.560	63.934	1.00	0.00	N
ATOM	3751	CA	ALA	279	106.300	72.479	64.659	1.00	0.00	C
ATOM	3752	C	ALA	279	107.139	71.631	65.676	1.00	0.00	C
ATOM	3753	O	ALA	279	106.714	71.487	66.822	1.00	0.00	O
ATOM	3754	CB	ALA	279	105.640	71.588	63.591	1.00	0.00	C
ATOM	3755	H	ALA	279	107.144	73.548	62.910	1.00	0.00	H
ATOM	3756	HA	ALA	279	105.486	72.953	65.245	1.00	0.00	H
ATOM	3757	2HB	ALA	279	105.033	72.162	62.868	1.00	0.00	H
ATOM	3758	3HB	ALA	279	106.390	71.021	63.011	1.00	0.00	H
ATOM	3759	1HB	ALA	279	104.968	70.841	64.053	1.00	0.00	H
ATOM	3760	N	SER	280	108.335	71.141	65.295	1.00	0.00	N
ATOM	3761	CA	SER	280	109.213	70.528	66.216	1.00	0.00	C
ATOM	3762	C	SER	280	109.772	71.215	67.465	1.00	0.00	C

ATOM	3774	O	LEU	281	109.153	74.008	70.512	0.00	0.00	O
ATOM	3775	CB	LEU	281	110.916	74.971	67.767	0.00	0.00	C
ATOM	3776	CG	LEU	281	111.466	76.022	68.769	0.00	0.00	C
ATOM	3777	CD1	LEU	281	112.724	75.538	69.510	0.00	0.00	C
ATOM	3778	CD2	LEU	281	111.794	77.333	68.038	0.00	0.00	C
ATOM	3779	H	LEU	281	110.044	73.008	66.280	0.00	0.00	H
ATOM	3780	HA	LEU	281	111.034	73.249	69.067	0.00	0.00	H
ATOM	3781	1HB	LEU	281	110.155	75.447	67.118	0.00	0.00	H
ATOM	3782	2HB	LEU	281	111.735	74.695	67.073	0.00	0.00	H
ATOM	3783	HG	LEU	281	110.686	76.238	69.526	0.00	0.00	H
ATOM	3784	1HD1	LEU	281	113.118	76.305	70.202	0.00	0.00	H
ATOM	3785	2HD1	LEU	281	112.523	74.639	70.123	0.00	0.00	H
ATOM	3786	3HD1	LEU	281	113.541	75.285	68.812	0.00	0.00	H
ATOM	3787	1HD2	LEU	281	112.150	78.116	68.736	0.00	0.00	H
ATOM	3788	2HD2	LEU	281	112.581	77.195	67.273	0.00	0.00	H
ATOM	3789	3HD2	LEU	281	110.909	77.749	67.522	0.00	0.00	H
ATOM	3790	N	ILE	282	107.811	74.141	68.710	1.00	0.00	N
ATOM	3791	CA	ILE	282	106.519	74.183	69.481	1.00	0.00	C
ATOM	3792	C	ILE	282	106.240	72.868	70.311	1.00	0.00	C
ATOM	3793	O	ILE	282	105.937	72.968	71.499	1.00	0.00	O
ATOM	3794	CB	ILE	282	105.333	74.624	68.532	1.00	0.00	C
ATOM	3795	CG1	ILE	282	105.508	76.060	67.944	1.00	0.00	C
ATOM	3796	CG2	ILE	282	103.939	74.566	69.215	1.00	0.00	C
ATOM	3797	CD1	ILE	282	104.640	76.398	66.716	1.00	0.00	C
ATOM	3798	H	ILE	282	107.829	74.102	67.681	1.00	0.00	H
ATOM	3799	HA	ILE	282	106.618	74.980	70.244	1.00	0.00	H
ATOM	3800	HB	ILE	282	105.319	73.908	67.686	1.00	0.00	H
ATOM	3801	1HG1	ILE	282	105.354	76.820	68.735	1.00	0.00	H
ATOM	3802	2HG1	ILE	282	106.559	76.201	67.631	1.00	0.00	H
ATOM	3803	2HG2	ILE	282	103.703	73.553	69.590	1.00	0.00	H
ATOM	3804	3HG2	ILE	282	103.874	75.257	70.076	1.00	0.00	H
ATOM	3805	1HG2	ILE	282	103.116	74.826	68.525	1.00	0.00	H
ATOM	3806	2HD1	ILE	282	104.804	75.679	65.892	1.00	0.00	H
ATOM	3807	3HD1	ILE	282	103.559	76.401	66.950	1.00	0.00	H
ATOM	3808	1HD1	ILE	282	104.881	77.403	66.322	1.00	0.00	H
ATOM	3809	N	GLN	283	106.365	71.662	69.727	1.00	0.00	N
ATOM	3810	CA	GLN	283	106.324	70.366	70.478	1.00	0.00	C
ATOM	3811	C	GLN	283	107.407	70.164	71.602	1.00	0.00	C
ATOM	3812	O	GLN	283	107.077	69.647	72.669	1.00	0.00	O
ATOM	3813	CB	GLN	283	106.371	69.207	69.441	1.00	0.00	C
ATOM	3814	CG	GLN	283	105.123	69.066	68.524	1.00	0.00	C
ATOM	3815	CD	GLN	283	105.263	67.998	67.437	1.00	0.00	C
ATOM	3816	OE1	GLN	283	105.841	68.208	66.378	1.00	0.00	O
ATOM	3817	NE2	GLN	283	104.736	66.821	67.648	1.00	0.00	N
ATOM	3818	H	GLN	283	106.619	71.701	68.728	1.00	0.00	H
ATOM	3819	HA	GLN	283	105.351	70.309	71.006	1.00	0.00	H
ATOM	3820	1HB	GLN	283	107.284	69.312	68.820	1.00	0.00	H
ATOM	3821	2HB	GLN	283	106.509	68.248	69.979	1.00	0.00	H
ATOM	3822	1HG	GLN	283	104.215	68.892	69.130	1.00	0.00	H
ATOM	3823	2HG	GLN	283	104.931	70.020	68.000	1.00	0.00	H
ATOM	3824	1HE2	GLN	283	104.316	66.660	68.566	1.00	0.00	H
ATOM	3825	2HE2	GLN	283	104.911	66.152	66.894	1.00	0.00	H
ATOM	3826	N	LYS	284	108.670	70.582	71.395	1.00	0.00	N
ATOM	3827	CA	LYS	284	109.702	70.663	72.477	1.00	0.00	C
ATOM	3828	C	LYS	284	109.350	71.603	73.689	1.00	0.00	C
ATOM	3829	O	LYS	284	109.483	71.189	74.843	1.00	0.00	O
ATOM	3830	CB	LYS	284	111.052	71.077	71.820	1.00	0.00	C
ATOM	3831	CG	LYS	284	111.752	69.995	70.965	1.00	0.00	C
ATOM	3832	CD	LYS	284	112.939	70.569	70.164	1.00	0.00	C
ATOM	3833	CE	LYS	284	113.574	69.518	69.246	1.00	0.00	C
ATOM	3834	NZ	LYS	284	114.669	70.131	68.468	1.00	0.00	N
ATOM	3835	1HZ	LYS	284	115.093	69.421	67.853	1.00	0.00	H
ATOM	3836	2HZ	LYS	284	114.295	70.901	67.895	1.00	0.00	H
ATOM	3837	3HZ	LYS	284	115.385	70.498	69.111	1.00	0.00	H
ATOM	3838	H	LYS	284	108.845	70.927	70.442	1.00	0.00	H
ATOM	3839	HA	LYS	284	109.825	69.652	72.914	1.00	0.00	H
ATOM	3840	1HB	LYS	284	110.891	71.994	71.217	1.00	0.00	H
ATOM	3841	2HB	LYS	284	111.762	71.394	72.606	1.00	0.00	H
ATOM	3842	1HG	LYS	284	112.088	69.161	71.612	1.00	0.00	H
ATOM	3843	2HG	LYS	284	111.023	69.541	70.266	1.00	0.00	H
ATOM	3844	1HD	LYS	284	112.585	71.426	69.555	1.00	0.00	H
ATOM	3845	2HD	LYS	284	113.695	70.985	70.860	1.00	0.00	H
ATOM	3846	1HE	LYS	284	113.956	68.663	69.840	1.00	0.00	H

ATOM	3847	2HE	LYS	284	112.813	69.091	68.562	1.00	0.00	H
ATOM	3848	N	MET	285	108.903	72.845	73.438	1.00	0.00	N
ATOM	3849	CA	MET	285	108.343	73.747	74.490	1.00	0.00	C
ATOM	3850	C	MET	285	107.007	73.268	75.172	1.00	0.00	C
ATOM	3851	O	MET	285	106.880	73.356	76.396	1.00	0.00	O
ATOM	3852	CB	MET	285	108.192	75.163	73.863	1.00	0.00	C
ATOM	3853	CG	MET	285	109.509	75.909	73.553	1.00	0.00	C
ATOM	3854	SD	MET	285	109.147	77.567	72.955	1.00	0.00	S
ATOM	3855	CE	MET	285	110.808	78.115	72.529	1.00	0.00	C
ATOM	3856	H	MET	285	108.820	73.061	72.436	1.00	0.00	H
ATOM	3857	HA	MET	285	109.080	73.822	75.315	1.00	0.00	H
ATOM	3858	1HB	MET	285	107.573	75.105	72.945	1.00	0.00	H
ATOM	3859	2HB	MET	285	107.603	75.796	74.550	1.00	0.00	H
ATOM	3860	1HG	MET	285	110.149	75.976	74.452	1.00	0.00	H
ATOM	3861	2HG	MET	285	110.091	75.364	72.785	1.00	0.00	H
ATOM	3862	1HE	MET	285	111.438	78.200	73.430	1.00	0.00	H
ATOM	3863	3HE	MET	285	111.288	77.407	71.829	1.00	0.00	H
ATOM	3864	2HE	MET	285	110.774	79.105	72.043	1.00	0.00	H
ATOM	3865	N	LEU	286	106.023	72.769	74.403	0.00	0.00	N
ATOM	3866	CA	LEU	286	104.734	72.249	74.938	0.00	0.00	C
ATOM	3867	C	LEU	286	104.765	70.689	75.136	0.00	0.00	C
ATOM	3868	O	LEU	286	104.191	69.933	74.344	0.00	0.00	O
ATOM	3869	CB	LEU	286	103.593	72.713	73.979	0.00	0.00	C
ATOM	3870	CG	LEU	286	103.350	74.234	73.781	0.00	0.00	C
ATOM	3871	CD1	LEU	286	102.345	74.488	72.647	0.00	0.00	C
ATOM	3872	CD2	LEU	286	102.828	74.911	75.053	0.00	0.00	C
ATOM	3873	H	LEU	286	106.248	72.721	73.399	0.00	0.00	H
ATOM	3874	HA	LEU	286	104.520	72.696	75.927	0.00	0.00	H
ATOM	3875	1HB	LEU	286	102.649	72.257	74.326	0.00	0.00	H
ATOM	3876	2HB	LEU	286	103.772	72.247	72.989	0.00	0.00	H
ATOM	3877	HG	LEU	286	104.310	74.702	73.489	0.00	0.00	H
ATOM	3878	1HD1	LEU	286	102.251	75.564	72.415	0.00	0.00	H
ATOM	3879	2HD1	LEU	286	102.649	73.981	71.715	0.00	0.00	H
ATOM	3880	3HD1	LEU	286	101.334	74.117	72.893	0.00	0.00	H
ATOM	3881	1HD2	LEU	286	102.662	75.994	74.907	0.00	0.00	H
ATOM	3882	2HD2	LEU	286	101.871	74.475	75.399	0.00	0.00	H
ATOM	3883	3HD2	LEU	286	103.544	74.819	75.886	0.00	0.00	H
ATOM	3884	N	GLN	287	105.413	70.203	76.211	0.00	0.00	N
ATOM	3885	CA	GLN	287	105.589	68.743	76.475	0.00	0.00	C
ATOM	3886	C	GLN	287	105.173	68.375	77.939	0.00	0.00	C
ATOM	3887	O	GLN	287	105.882	68.685	78.895	0.00	0.00	O
ATOM	3888	CB	GLN	287	107.068	68.397	76.131	0.00	0.00	C
ATOM	3889	CG	GLN	287	107.540	66.935	76.360	0.00	0.00	C
ATOM	3890	CD	GLN	287	106.894	65.837	75.513	0.00	0.00	C
ATOM	3891	OE1	GLN	287	107.388	65.437	74.467	0.00	0.00	O
ATOM	3892	NE2	GLN	287	105.791	65.276	75.937	0.00	0.00	N
ATOM	3893	H	GLN	287	105.978	70.908	76.702	0.00	0.00	H
ATOM	3894	HA	GLN	287	104.957	68.147	75.785	0.00	0.00	H
ATOM	3895	1HB	GLN	287	107.737	69.060	76.715	0.00	0.00	H
ATOM	3896	2HB	GLN	287	107.271	68.671	75.076	0.00	0.00	H
ATOM	3897	1HG	GLN	287	107.477	66.675	77.433	0.00	0.00	H
ATOM	3898	2HG	GLN	287	108.623	66.896	76.145	0.00	0.00	H
ATOM	3899	1HE2	GLN	287	105.310	65.754	76.700	0.00	0.00	H
ATOM	3900	2HE2	GLN	287	105.393	64.634	75.247	0.00	0.00	H
ATOM	3901	N	THR	288	104.048	67.664	78.139	1.00	0.00	N
ATOM	3902	CA	THR	288	103.543	67.291	79.511	1.00	0.00	C
ATOM	3903	C	THR	288	104.436	66.358	80.418	1.00	0.00	C
ATOM	3904	O	THR	288	104.234	66.308	81.634	1.00	0.00	O
ATOM	3905	CB	THR	288	102.058	66.822	79.200	1.00	0.00	C
ATOM	3906	OG1	THR	288	101.434	66.860	80.660	1.00	0.00	O
ATOM	3907	CG2	THR	288	101.822	65.303	78.615	1.00	0.00	C
ATOM	3908	H	THR	288	103.113	67.701	77.290	1.00	0.00	H
ATOM	3909	HA	THR	288	103.644	68.222	80.011	1.00	0.00	H
ATOM	3910	HB	THR	288	101.613	67.000	78.615	1.00	0.00	H

ATOM	3920	CG	ASP	289	105.899	62.579	79.992	0.00	0.00	C
ATOM	3921	OD1	ASP	289	105.743	61.857	80.970	0.00	0.00	O
ATOM	3922	OD2	ASP	289	105.173	62.469	78.848	0.00	0.00	O
ATOM	3923	H	ASP	289	105.566	65.931	78.873	0.00	0.00	H
ATOM	3924	HA	ASP	289	106.183	64.747	81.643	0.00	0.00	H
ATOM	3925	1HB	ASP	289	107.856	63.302	80.362	0.00	0.00	H
ATOM	3926	2HB	ASP	289	107.206	63.884	78.866	0.00	0.00	H
ATOM	3927	N	PRO	290	108.009	66.769	81.862	1.00	0.00	N
ATOM	3928	CA	PRO	290	109.137	67.754	81.926	1.00	0.00	C
ATOM	3929	C	PRO	290	110.615	67.241	81.787	1.00	0.00	C
ATOM	3930	O	PRO	290	111.483	68.016	81.382	1.00	0.00	O
ATOM	3931	CB	PRO	290	108.847	68.505	83.240	1.00	0.00	C
ATOM	3932	CG	PRO	290	107.998	67.547	84.076	1.00	0.00	C
ATOM	3933	CD	PRO	290	107.135	66.813	83.051	1.00	0.00	C
ATOM	3934	HA	PRO	290	109.003	68.477	81.096	1.00	0.00	H
ATOM	3935	1HB	PRO	290	109.761	68.838	83.770	1.00	0.00	H
ATOM	3936	2HB	PRO	290	108.273	69.427	83.016	1.00	0.00	H
ATOM	3937	1HG	PRO	290	108.650	66.830	84.612	1.00	0.00	H
ATOM	3938	2HG	PRO	290	107.394	68.066	84.842	1.00	0.00	H
ATOM	3939	1HD	PRO	290	106.837	65.816	83.426	1.00	0.00	H
ATOM	3940	2HD	PRO	290	106.212	67.384	82.828	1.00	0.00	H
ATOM	3941	N	THR	291	110.902	65.954	82.033	0.00	0.00	N
ATOM	3942	CA	THR	291	112.170	65.287	81.572	0.00	0.00	C
ATOM	3943	C	THR	291	112.443	65.277	80.021	0.00	0.00	C
ATOM	3944	O	THR	291	113.599	65.396	79.608	0.00	0.00	O
ATOM	3945	CB	THR	291	112.272	63.838	82.150	0.00	0.00	C
ATOM	3946	OG1	THR	291	111.144	63.050	81.782	0.00	0.00	O
ATOM	3947	CG2	THR	291	112.401	63.745	83.679	0.00	0.00	C
ATOM	3948	H	THR	291	110.076	65.407	82.290	0.00	0.00	H
ATOM	3949	HA	THR	291	113.018	65.861	81.998	0.00	0.00	H
ATOM	3950	HB	THR	291	113.182	63.366	81.723	0.00	0.00	H
ATOM	3951	HG1	THR	291	111.255	62.203	82.220	0.00	0.00	H
ATOM	3952	1HG2	THR	291	112.536	62.702	84.020	0.00	0.00	H
ATOM	3953	2HG2	THR	291	113.270	64.321	84.048	0.00	0.00	H
ATOM	3954	3HG2	THR	291	111.506	64.145	84.192	0.00	0.00	H
ATOM	3955	N	ALA	292	111.407	65.155	79.170	1.00	0.00	N
ATOM	3956	CA	ALA	292	111.517	65.430	77.707	1.00	0.00	C
ATOM	3957	C	ALA	292	111.351	66.921	77.217	1.00	0.00	C
ATOM	3958	O	ALA	292	111.419	67.163	76.008	1.00	0.00	O
ATOM	3959	CB	ALA	292	110.464	64.496	77.075	1.00	0.00	C
ATOM	3960	H	ALA	292	110.496	65.160	79.642	1.00	0.00	H
ATOM	3961	HA	ALA	292	112.511	65.107	77.339	1.00	0.00	H
ATOM	3962	2HB	ALA	292	110.646	63.432	77.318	1.00	0.00	H
ATOM	3963	3HB	ALA	292	109.436	64.743	77.400	1.00	0.00	H
ATOM	3964	1HB	ALA	292	110.472	64.572	75.971	1.00	0.00	H
ATOM	3965	N	ARG	293	111.155	67.913	78.102	0.00	0.00	N
ATOM	3966	CA	ARG	293	111.035	69.349	77.730	0.00	0.00	C
ATOM	3967	C	ARG	293	112.431	70.079	77.848	0.00	0.00	C
ATOM	3968	O	ARG	293	112.874	70.307	78.980	0.00	0.00	O
ATOM	3969	CB	ARG	293	109.945	69.948	78.668	0.00	0.00	C
ATOM	3970	CG	ARG	293	109.355	71.322	78.250	0.00	0.00	C
ATOM	3971	CD	ARG	293	108.545	72.043	79.350	0.00	0.00	C
ATOM	3972	NE	ARG	293	107.377	71.246	79.800	0.00	0.00	N
ATOM	3973	CZ	ARG	293	106.613	71.500	80.849	0.00	0.00	C
ATOM	3974	NH1	ARG	293	106.746	72.531	81.627	0.00	0.00	N
ATOM	3975	NH2	ARG	293	105.679	70.655	81.106	0.00	0.00	N
ATOM	3976	HE	ARG	293	107.138	70.414	79.242	1.00	0.00	H
ATOM	3977	H	ARG	293	111.190	67.608	79.081	0.00	0.00	H
ATOM	3978	HA	ARG	293	110.638	69.440	76.702	0.00	0.00	H
ATOM	3979	1HB	ARG	293	110.346	70.018	79.696	0.00	0.00	H
ATOM	3980	2HB	ARG	293	109.087	69.250	78.757	0.00	0.00	H
ATOM	3981	1HG	ARG	293	108.717	71.197	77.352	0.00	0.00	H
ATOM	3982	2HG	ARG	293	110.172	71.994	77.921	0.00	0.00	H
ATOM	3983	1HD	ARG	293	108.180	73.013	78.961	0.00	0.00	H
ATOM	3984	2HD	ARG	293	109.216	72.282	80.197	0.00	0.00	H
ATOM	3985	1HH1	ARG	293	106.110	72.599	82.417	0.00	0.00	H
ATOM	3986	2HH1	ARG	293	107.501	73.161	81.338	0.00	0.00	H
ATOM	3987	1HH2	ARG	293	105.098	70.793	81.925	0.00	0.00	H
ATOM	3988	2HH2	ARG	293	105.711	69.884	80.425	0.00	0.00	H
ATOM	3989	N	PRO	294	113.176	70.471	76.769	1.00	0.00	N
ATOM	3990	CA	PRO	294	114.485	71.175	76.914	1.00	0.00	C
ATOM	3991	C	PRO	294	114.392	72.639	77.466	1.00	0.00	C
ATOM	3992	O	PRO	294	113.468	73.393	77.152	1.00	0.00	O

ATOM	3993	CB	PRO	294	115.049	71.081	75.481	1.00	0.00	C
ATOM	3994	CG	PRO	294	113.832	70.955	74.566	1.00	0.00	C
ATOM	3995	CD	PRO	294	112.832	70.136	75.375	1.00	0.00	C
ATOM	3996	HA	PRO	294	115.134	70.581	77.588	1.00	0.00	H
ATOM	3997	1HB	PRO	294	115.680	71.944	75.202	1.00	0.00	H
ATOM	3998	2HB	PRO	294	115.686	70.180	75.389	1.00	0.00	H
ATOM	3999	1HG	PRO	294	113.411	71.958	74.363	1.00	0.00	H
ATOM	4000	2HG	PRO	294	114.067	70.495	73.588	1.00	0.00	H
ATOM	4001	1HD	PRO	294	111.795	70.403	75.105	1.00	0.00	H
ATOM	4002	2HD	PRO	294	112.957	69.050	75.192	1.00	0.00	H
ATOM	4003	N	THR	295	115.339	73.037	78.328	1.00	0.00	N
ATOM	4004	CA	THR	295	115.353	74.386	78.981	1.00	0.00	C
ATOM	4005	C	THR	295	116.817	74.695	79.466	1.00	0.00	C
ATOM	4006	O	THR	295	117.387	73.917	80.231	1.00	0.00	O
ATOM	4007	CB	THR	295	114.333	74.468	80.166	1.00	0.00	C
ATOM	4008	OG1	THR	295	113.010	74.194	79.725	1.00	0.00	O
ATOM	4009	CG2	THR	295	114.231	75.846	80.832	1.00	0.00	C
ATOM	4010	H	THR	295	116.015	72.303	78.578	1.00	0.00	H
ATOM	4011	HA	THR	295	115.040	75.133	78.232	1.00	0.00	H
ATOM	4012	HB	THR	295	114.610	73.714	80.932	1.00	0.00	H
ATOM	4013	HG1	THR	295	113.092	73.632	78.939	1.00	0.00	H
ATOM	4014	1HG2	THR	295	113.968	76.636	80.108	1.00	0.00	H
ATOM	4015	2HG2	THR	295	113.451	75.851	81.616	1.00	0.00	H
ATOM	4016	3HG2	THR	295	115.181	76.140	81.311	1.00	0.00	H
ATOM	4017	N	ILE	296	117.571	75.760	79.174	1.00	0.00	N
ATOM	4018	CA	ILE	296	117.200	76.943	78.320	1.00	0.00	C
ATOM	4019	C	ILE	296	118.198	77.193	77.130	1.00	0.00	C
ATOM	4020	O	ILE	296	117.754	77.424	76.002	1.00	0.00	O
ATOM	4021	CB	ILE	296	116.909	78.203	79.219	1.00	0.00	C
ATOM	4022	CG1	ILE	296	116.285	79.421	78.478	1.00	0.00	C
ATOM	4023	CG2	ILE	296	118.123	78.712	80.038	1.00	0.00	C
ATOM	4024	CD1	ILE	296	114.886	79.182	77.886	1.00	0.00	C
ATOM	4025	H	ILE	296	118.460	75.689	79.683	1.00	0.00	H
ATOM	4026	HA	ILE	296	116.253	76.730	77.797	1.00	0.00	H
ATOM	4027	HB	ILE	296	116.153	77.880	79.960	1.00	0.00	H
ATOM	4028	1HG1	ILE	296	116.200	80.276	79.177	1.00	0.00	H
ATOM	4029	2HG1	ILE	296	116.970	79.783	77.684	1.00	0.00	H
ATOM	4030	2HG2	ILE	296	118.571	77.916	80.662	1.00	0.00	H
ATOM	4031	3HG2	ILE	296	118.925	79.109	79.388	1.00	0.00	H
ATOM	4032	1HG2	ILE	296	117.843	79.526	80.735	1.00	0.00	H
ATOM	4033	2HD1	ILE	296	114.897	78.440	77.066	1.00	0.00	H
ATOM	4034	3HD1	ILE	296	114.170	78.831	78.652	1.00	0.00	H
ATOM	4035	1HD1	ILE	296	114.472	80.115	77.461	1.00	0.00	H
ATOM	4036	N	ASN	297	119.524	77.082	77.342	1.00	0.00	N
ATOM	4037	CA	ASN	297	120.539	76.963	76.244	1.00	0.00	C
ATOM	4038	C	ASN	297	120.318	75.865	75.137	1.00	0.00	C
ATOM	4039	O	ASN	297	120.720	76.074	73.993	1.00	0.00	O
ATOM	4040	CB	ASN	297	121.955	76.877	76.885	1.00	0.00	C
ATOM	4041	CG	ASN	297	122.271	75.635	77.728	1.00	0.00	C
ATOM	4042	OD1	ASN	297	121.591	75.318	78.696	1.00	0.00	O
ATOM	4043	ND2	ASN	297	123.300	74.896	77.410	1.00	0.00	N
ATOM	4044	H	ASN	297	119.777	76.885	78.316	1.00	0.00	H
ATOM	4045	HA	ASN	297	120.509	77.926	75.696	1.00	0.00	H
ATOM	4046	1HB	ASN	297	122.710	77.007	76.087	1.00	0.00	H
ATOM	4047	2HB	ASN	297	122.116	77.751	77.540	1.00	0.00	H
ATOM	4048	1HD2	ASN	297	123.467	74.122	78.059	1.00	0.00	H
ATOM	4049	2HD2	ASN	297	123.883	75.208	76.631	1.00	0.00	H
ATOM	4050	N	GLU	298	119.665	74.735	75.458	1.00	0.00	N
ATOM	4051	CA	GLU	298	119.131	73.759	74.458	1.00	0.00	C
ATOM	4052	C	GLU	298	118.095	74.333	73.417	1.00	0.00	C
ATOM	4053	O	GLU	298	118.222	74.070	72.223	1.00	0.00	C
ATOM	4054	CB	GLU	298	118.500	72.575	75.247	1.00	0.00	C

ATOM	4066	CA	LEU	299	116.186	75.882	72.942	1.00	0.00	C
ATOM	4067	C	LEU	299	116.861	77.050	72.136	1.00	0.00	C
ATOM	4068	O	LEU	299	116.532	77.249	70.965	1.00	0.00	O
ATOM	4069	CB	LEU	299	114.977	76.408	73.767	1.00	0.00	C
ATOM	4070	CG	LEU	299	113.984	75.356	74.328	1.00	0.00	C
ATOM	4071	CD1	LEU	299	113.061	76.019	75.358	1.00	0.00	C
ATOM	4072	CD2	LEU	299	113.127	74.708	73.229	1.00	0.00	C
ATOM	4073	H	LEU	299	117.153	75.335	74.857	1.00	0.00	H
ATOM	4074	HA	LEU	299	115.798	75.187	72.171	1.00	0.00	H
ATOM	4075	1HB	LEU	299	115.370	77.032	74.594	1.00	0.00	H
ATOM	4076	2HB	LEU	299	114.398	77.123	73.148	1.00	0.00	H
ATOM	4077	HG	LEU	299	114.545	74.556	74.851	1.00	0.00	H
ATOM	4078	2HD1	LEU	299	113.638	76.425	76.207	1.00	0.00	H
ATOM	4079	3HD1	LEU	299	112.472	76.850	74.931	1.00	0.00	H
ATOM	4080	1HD1	LEU	299	112.342	75.295	75.786	1.00	0.00	H
ATOM	4081	2HD2	LEU	299	112.564	75.457	72.642	1.00	0.00	H
ATOM	4082	3HD2	LEU	299	113.738	74.125	72.517	1.00	0.00	H
ATOM	4083	1HD2	LEU	299	112.380	74.008	73.649	1.00	0.00	H
ATOM	4084	N	LEU	300	117.800	77.804	72.742	0.00	0.00	N
ATOM	4085	CA	LEU	300	118.689	78.749	72.003	0.00	0.00	C
ATOM	4086	C	LEU	300	119.619	78.094	70.910	0.00	0.00	C
ATOM	4087	O	LEU	300	119.696	78.602	69.791	0.00	0.00	O
ATOM	4088	CB	LEU	300	119.475	79.548	73.087	0.00	0.00	C
ATOM	4089	CG	LEU	300	120.146	80.865	72.617	0.00	0.00	C
ATOM	4090	CD1	LEU	300	119.115	81.989	72.419	0.00	0.00	C
ATOM	4091	CD2	LEU	300	121.191	81.327	73.645	0.00	0.00	C
ATOM	4092	H	LEU	300	117.959	77.545	73.722	0.00	0.00	H
ATOM	4093	HA	LEU	300	118.035	79.456	71.458	0.00	0.00	H
ATOM	4094	1HB	LEU	300	120.243	78.874	73.511	0.00	0.00	H
ATOM	4095	2HB	LEU	300	118.821	79.790	73.950	0.00	0.00	H
ATOM	4096	HG	LEU	300	120.669	80.685	71.654	0.00	0.00	H
ATOM	4097	1HD1	LEU	300	119.592	82.917	72.055	0.00	0.00	H
ATOM	4098	2HD1	LEU	300	118.343	81.724	71.675	0.00	0.00	H
ATOM	4099	3HD1	LEU	300	118.589	82.249	73.357	0.00	0.00	H
ATOM	4100	1HD2	LEU	300	121.695	82.259	73.327	0.00	0.00	H
ATOM	4101	2HD2	LEU	300	120.746	81.517	74.640	0.00	0.00	H
ATOM	4102	3HD2	LEU	300	121.988	80.573	73.783	0.00	0.00	H
ATOM	4103	N	ASN	301	120.297	76.970	71.206	1.00	0.00	N
ATOM	4104	CA	ASN	301	121.104	76.208	70.204	1.00	0.00	C
ATOM	4105	C	ASN	301	120.227	75.154	69.432	1.00	0.00	C
ATOM	4106	O	ASN	301	120.271	73.949	69.696	1.00	0.00	O
ATOM	4107	CB	ASN	301	122.318	75.573	70.940	1.00	0.00	C
ATOM	4108	CG	ASN	301	123.381	76.548	71.451	1.00	0.00	C
ATOM	4109	OD1	ASN	301	124.255	77.005	70.727	1.00	0.00	O
ATOM	4110	ND2	ASN	301	123.349	76.909	72.706	1.00	0.00	N
ATOM	4111	H	ASN	301	120.089	76.589	72.137	1.00	0.00	H
ATOM	4112	HA	ASN	301	121.521	76.899	69.441	1.00	0.00	H
ATOM	4113	1HB	ASN	301	121.973	74.907	71.753	1.00	0.00	H
ATOM	4114	2HB	ASN	301	122.841	74.896	70.241	1.00	0.00	H
ATOM	4115	1HD2	ASN	301	124.007	77.663	72.912	1.00	0.00	H
ATOM	4116	2HD2	ASN	301	122.480	76.659	73.193	1.00	0.00	H
ATOM	4117	N	ASP	302	119.431	75.633	68.462	1.00	0.00	N
ATOM	4118	CA	ASP	302	118.470	74.800	67.682	1.00	0.00	C
ATOM	4119	C	ASP	302	118.558	75.124	66.146	1.00	0.00	C
ATOM	4120	O	ASP	302	118.888	76.244	65.746	1.00	0.00	O
ATOM	4121	CB	ASP	302	117.068	75.070	68.304	1.00	0.00	C
ATOM	4122	CG	ASP	302	115.930	74.205	67.769	1.00	0.00	C
ATOM	4123	OD1	ASP	302	115.315	74.453	66.736	1.00	0.00	O
ATOM	4124	OD2	ASP	302	115.684	73.122	68.555	1.00	0.00	O
ATOM	4125	H	ASP	302	119.450	76.657	68.388	1.00	0.00	H
ATOM	4126	HA	ASP	302	118.713	73.724	67.810	1.00	0.00	H
ATOM	4127	1HB	ASP	302	117.108	74.932	69.403	1.00	0.00	H
ATOM	4128	2HB	ASP	302	116.784	76.131	68.168	1.00	0.00	H
ATOM	4129	N	GLU	303	118.186	74.166	65.272	1.00	0.00	N
ATOM	4130	CA	GLU	303	118.106	74.393	63.789	1.00	0.00	C
ATOM	4131	C	GLU	303	117.247	75.612	63.272	1.00	0.00	C
ATOM	4132	O	GLU	303	117.653	76.272	62.311	1.00	0.00	O
ATOM	4133	CB	GLU	303	117.698	73.037	63.143	1.00	0.00	C
ATOM	4134	CG	GLU	303	117.791	72.950	61.594	1.00	0.00	C
ATOM	4135	CD	GLU	303	119.196	73.093	61.008	1.00	0.00	C
ATOM	4136	OE1	GLU	303	120.002	72.174	60.934	1.00	0.00	O
ATOM	4137	OE2	GLU	303	119.453	74.358	60.580	1.00	0.00	O
ATOM	4138	H	GLU	303	117.932	73.274	65.704	1.00	0.00	H

ATOM	4139	HA	GLU	303	119.138	74.609	63.453	1.00	0.00	H
ATOM	4140	1HB	GLU	303	118.319	72.218	63.562	1.00	0.00	H
ATOM	4141	2HB	GLU	303	116.662	72.789	63.449	1.00	0.00	H
ATOM	4142	1HG	GLU	303	117.397	71.974	61.259	1.00	0.00	H
ATOM	4143	2HG	GLU	303	117.126	73.698	61.122	1.00	0.00	H
ATOM	4144	N	PHE	304	116.123	75.957	63.930	1.00	0.00	N
ATOM	4145	CA	PHE	304	115.408	77.255	63.706	1.00	0.00	C
ATOM	4146	C	PHE	304	116.187	78.601	64.004	1.00	0.00	C
ATOM	4147	O	PHE	304	115.678	79.671	63.666	1.00	0.00	O
ATOM	4148	CB	PHE	304	114.086	77.155	64.532	1.00	0.00	C
ATOM	4149	CG	PHE	304	112.952	78.103	64.094	1.00	0.00	C
ATOM	4150	CD1	PHE	304	112.209	77.828	62.941	1.00	0.00	C
ATOM	4151	CE1	PHE	304	111.199	78.696	62.531	1.00	0.00	C
ATOM	4152	CZ	PHE	304	110.911	79.832	63.280	1.00	0.00	C
ATOM	4153	CE2	PHE	304	111.637	80.110	64.436	1.00	0.00	C
ATOM	4154	CD2	PHE	304	112.654	79.248	64.842	1.00	0.00	C
ATOM	4155	H	PHE	304	115.943	75.378	64.761	1.00	0.00	H
ATOM	4156	HA	PHE	304	115.142	77.303	62.631	1.00	0.00	H
ATOM	4157	1HB	PHE	304	113.671	76.131	64.512	1.00	0.00	H
ATOM	4158	2HB	PHE	304	114.322	77.303	65.605	1.00	0.00	H
ATOM	4159	HD1	PHE	304	112.421	76.945	62.353	1.00	0.00	H
ATOM	4160	HE1	PHE	304	110.639	78.489	61.632	1.00	0.00	H
ATOM	4161	HZ	PHE	304	110.124	80.503	62.962	1.00	0.00	H
ATOM	4162	HE2	PHE	304	111.414	80.993	65.017	1.00	0.00	H
ATOM	4163	HD2	PHE	304	113.223	79.482	65.731	1.00	0.00	H
ATOM	4164	N	PHE	305	117.381	78.573	64.630	1.00	0.00	N
ATOM	4165	CA	PHE	305	118.152	79.787	65.016	1.00	0.00	C
ATOM	4166	C	PHE	305	119.662	79.644	64.585	1.00	0.00	C
ATOM	4167	O	PHE	305	120.540	79.402	65.413	1.00	0.00	O
ATOM	4168	CB	PHE	305	117.850	80.000	66.535	1.00	0.00	C
ATOM	4169	CG	PHE	305	118.007	81.423	67.096	1.00	0.00	C
ATOM	4170	CD1	PHE	305	117.364	82.517	66.501	1.00	0.00	C
ATOM	4171	CE1	PHE	305	117.504	83.793	67.039	1.00	0.00	C
ATOM	4172	CZ	PHE	305	118.254	83.979	68.198	1.00	0.00	C
ATOM	4173	CE2	PHE	305	118.865	82.894	68.816	1.00	0.00	C
ATOM	4174	CD2	PHE	305	118.748	81.623	68.264	1.00	0.00	C
ATOM	4175	H	PHE	305	117.712	77.629	64.875	1.00	0.00	H
ATOM	4176	HA	PHE	305	117.765	80.671	64.481	1.00	0.00	H
ATOM	4177	1HB	PHE	305	116.802	79.722	66.766	1.00	0.00	H
ATOM	4178	2HB	PHE	305	118.447	79.271	67.120	1.00	0.00	H
ATOM	4179	HD1	PHE	305	116.765	82.390	65.609	1.00	0.00	H
ATOM	4180	HE1	PHE	305	117.030	84.635	66.552	1.00	0.00	H
ATOM	4181	HZ	PHE	305	118.367	84.968	68.618	1.00	0.00	H
ATOM	4182	HE2	PHE	305	119.442	83.036	69.715	1.00	0.00	H
ATOM	4183	HD2	PHE	305	119.245	80.795	68.747	1.00	0.00	H
ATOM	4184	N	THR	306	119.955	79.784	63.270	1.00	0.00	N
ATOM	4185	CA	THR	306	121.282	79.388	62.661	1.00	0.00	C
ATOM	4186	C	THR	306	122.021	80.408	61.698	1.00	0.00	C
ATOM	4187	O	THR	306	123.248	80.336	61.626	1.00	0.00	O
ATOM	4188	CB	THR	306	121.171	77.981	61.978	1.00	0.00	C
ATOM	4189	OG1	THR	306	120.041	77.881	61.114	1.00	0.00	O
ATOM	4190	CG2	THR	306	121.072	76.801	62.954	1.00	0.00	C
ATOM	4191	H	THR	306	119.106	79.752	62.694	1.00	0.00	H
ATOM	4192	HA	THR	306	122.024	79.272	63.477	1.00	0.00	H
ATOM	4193	HB	THR	306	122.083	77.809	61.368	1.00	0.00	H
ATOM	4194	HG1	THR	306	119.374	77.379	61.601	1.00	0.00	H
ATOM	4195	1HG2	THR	306	121.035	75.832	62.425	1.00	0.00	H
ATOM	4196	2HG2	THR	306	121.942	76.765	63.637	1.00	0.00	H
ATOM	4197	3HG2	THR	306	120.171	76.867	62.221	1.00	0.00	H
ATOM	4198	N	SER	307	121.351	81.322	60.959	1.00	0.00	N
ATOM	4199	CA	SER	307	122.008	82.379	60.065	1.00	0.00	C
ATOM	4200	C	SER	307	121.211	82.703	58.803	1.00	0.00	C
ATOM	4201	O	SER	307	121.781	83.211	57.837	1.00	0.00	O
ATOM	4202	CB	SER	307	122.211	83.644	60.911	1.00	0.00	C
ATOM	4203	OG	SER	307	123.111	83.411	61.981	1.00	0.00	O
ATOM	4204	H	SER	307	120.351	81.322	60.959	1.00	0.00	H
ATOM	4205	HA	SER	307	122.008	82.379	60.065	1.00	0.00	H
ATOM	4206	HB2	SER	307	122.211	83.644	60.911	1.00	0.00	H
ATOM	4207	HB3	SER	307	123.111	83.411	61.981	1.00	0.00	H
ATOM	4208	HG	SER	307	123.111	83.411	61.981	1.00	0.00	H

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ATOM   4212  OC  GLY   308     121.218  87.503  62.866  1.00  0.00           O
ATOM   4213  O   GLY   308     122.904  87.719  61.299  0.00  0.00           O
ATOM   4214  HC  GLY   308     120.660  86.703  63.195  1.00  0.00           H
ATOM   4215  H   GLY   308     122.592  84.429  61.338  1.00  0.00           H
ATOM   4216 1HA  GLY   308     121.270  86.515  59.672  0.00  0.00           H
ATOM   4217 2HA  GLY   308     120.155  86.006  60.912  0.00  0.00           H
TER
ATOM   4218  PG  ATP   400H     94.957  91.733  84.664  1.00 56.62           P
ATOM   4219  O1G ATP   400H     94.187  90.944  83.509  1.00 61.42           O
ATOM   4220  PB  ATP   400H     95.915  93.870  83.671  1.00 53.17           P
ATOM   4221  O1B ATP   400H     96.089  93.010  82.330  1.00 54.96           O
ATOM   4222  O1A ATP   400H     96.187  97.690  82.708  1.00 34.47           O
ATOM   4223  PA  ATP   400H     96.566  96.129  82.542  1.00 45.52           P
ATOM   4224  O5  ATP   400H     98.142  95.970  82.935  1.00 43.48           O
ATOM   4225  O3B ATP   400H     94.875  93.256  84.560  1.00 53.99           O
ATOM   4226  O2G ATP   400H     96.437  91.126  84.983  1.00 57.35           O
ATOM   4227  O3G ATP   400H     94.312  91.481  86.097  1.00 57.62           O
ATOM   4228  O2A ATP   400H     96.428  95.839  80.960  1.00 42.48           O
ATOM   4229  O3A ATP   400H     95.542  95.326  83.388  1.00 50.69           O
ATOM   4230  O2B ATP   400H     97.232  93.930  84.606  1.00 58.07           O
ATOM   4231  C5A ATP   400H     99.030  97.140  83.056  1.00 39.42           C
ATOM   4232  C5  ATP   400H    105.482  98.998  81.874  1.00 22.15           C
ATOM   4233  O2  ATP   400H    102.885  98.017  86.127  1.00 41.77           O
ATOM   4234  C2A ATP   400H    102.084  98.131  84.952  1.00 38.93           C
ATOM   4235  C2  ATP   400H    103.750 100.569  80.504  1.00 24.73           C
ATOM   4236  O4  ATP   400H    101.513  97.285  82.879  1.00 32.13           O
ATOM   4237  C1  ATP   400H    102.647  97.361  83.759  1.00 30.56           C
ATOM   4238  N9  ATP   400H    103.870  98.006  83.189  1.00 23.28           N
ATOM   4239  C8  ATP   400H    105.187  97.588  83.362  1.00 19.33           C
ATOM   4240  N7  ATP   400H    106.229  98.104  82.631  1.00 24.44           N
ATOM   4241  C4  ATP   400H    104.058  98.982  82.211  1.00 23.86           C
ATOM   4242  C6  ATP   400H    105.895  99.858  80.790  1.00 20.25           C
ATOM   4243  N6  ATP   400H    107.148  99.906  80.376  1.00 24.16           N
ATOM   4244  N1  ATP   400H    105.019 100.612  80.163  1.00 22.35           N
ATOM   4245  N3  ATP   400H    103.170  99.872  81.450  1.00 25.23           N
ATOM   4246  O3  ATP   400H    100.578  96.609  86.178  1.00 49.35           O
ATOM   4247  C3  ATP   400H    100.670  97.532  85.088  1.00 39.09           C
ATOM   4248  C4A ATP   400H    100.405  96.839  83.718  1.00 36.99           C
ATOM   4249 2H5  ATP   400H     99.210  97.562  82.051  1.00  0.00           H
ATOM   4250 1H5  ATP   400H     98.505  97.953  83.587  1.00  0.00           H
ATOM   4251  H2A ATP   400H    102.013  99.195  84.663  1.00  0.00           H
ATOM   4252  H2  ATP   400H    103.102 101.207  79.921  1.00  0.00           H
ATOM   4253  H1  ATP   400H    102.912  96.326  84.052  1.00  0.00           H
ATOM   4254  H8  ATP   400H    105.406  96.787  84.057  1.00  0.00           H
ATOM   4255 1H6  ATP   400H    107.816  99.359  80.926  1.00  0.00           H
ATOM   4256 2H6  ATP   400H    107.380 100.761  79.847  1.00  0.00           H
ATOM   4257  HO2 ATP   400H    103.375  97.170  86.050  1.00  0.00           H
ATOM   4258  HO3 ATP   400H    101.361  96.023  86.141  1.00  0.00           H
ATOM   4259  H3  ATP   400H     99.958  98.359  85.265  1.00  0.00           H
ATOM   4260  H4  ATP   400H    100.487  95.738  83.832  1.00  0.00           H
END
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Table 3. Inhibition of PLK1 enzymatic activity by adenosine, thioadenosines, and various thiol-reactive compounds in the presence or absence of dithiothreitol (+DTT or –DTT); IC_{50}; concentration with half-maximal inhibition.

Compound	IC_{50} (μM)	
	+ DTT	*- DTT*
Thimerosal	> 200	22
N-ethylmaleimide	> 200	55
Iodoacetamide	> 200	83
Adenosine	> 200	> 200
2'-Thioadenosine	> 200	120
5'-Thioadenosine	> 200	39

Table 4. PLK1 contact model (Maestro) for ATP.

PLK1		ATP atom	Distance (Å)	Contact cut-off ratio
Residue	*Atom*			
K178	NZ	O1B	3.1	1.0
K178	CE	O1B	4.0	1.2
R135	NH1	O1A	3.9	1.2
K61	CA	O1A	4.2	1.3
K61	N	O1A	3.0	1.0
G60	N	O1A	4.1	1.3
G60	C	O1A	3.2	1.0
R135	NH1	PA	3.3	1.0
R135	CZ	PA	4.3	1.2
G60	3HD2	PA	4.4	1.3
R135	NH1	O5	3.1	1.0
G63	N	O3G	3.9	1.2
R135	NE	O2A	3.9	1.2
F135	NH2	O2A	3.3	1.0
R136	CZ	O2A	3.0	0.9
F136	NH1	C5A	3.3	1.0
C67	SG	C5A	3.7	1.1
F133	CE2	C5	4.0	1

D194	CG	O2	3.2	1.0
K82	NZ	O2	3.4	1.1
K82	CE	O2	3.3	1.0
K82	CD	O2	3.3	1.0
K82	CG	O2	4.1	1.3
K82	CB	O2	3.9	1.2
C67	SG	C2A	4.1	1.2
D194	OD2	C2A	3.4	1.1
D194	OD1	C2A	3.6	1.1
D194	CG	C2A	3.8	1.1
K82	CD	C2A	4.4	1.3
C67	CB	C2A	3.9	1.1
F183	CZ	C2	4.6	1.3
F183	CE1	C2	3.7	1.0
F183	CD1	C2	3.9	1.1
C133	O	C2	3.4	1.0
C133	C	C2	4.4	1.3
A80	CB	C2	3.4	1.0
L59	CD1	C2	4.3	1.2
L59	CG	C2	4.4	1.3
C67	SG	O4	4.2	1.3
F183	CZ	O4	3.6	1.1
F183	CE1	O4	4.0	1.2
D194	CB	C1	4.4	1.3
F183	CZ	C1	3.8	1.1
F183	CE1	C1	4.4	1.3
D194	OD2	C1	3.3	1.0
D194	OD1	C1	3.8	1.1
D194	CG	C1	3.6	1.0
F183	CE2	N9	4.0	1.2
F183	CZ	N9	3.5	1.0
F183	CE1	N9	3.8	1.2
D194	OD2	N9	3.7	1.2
D194	CG	N9	4.3	1.3
D194	CB	C8	4.5	1.3
F183	CE2	C8	3.7	1.1
F183	CZ	C8	3.7	1.0
F183	CE1	C8	4.2	1.2
D194	OD2	C8	3.4	1.0
D194	CG	C8	4.1	1.2
G193	C	C8	4.1	1.2
G193	C	C8	4.3	1.2
D194	N	C8	3.9	1.2
F183	CD2	C8	4.4	1.2
L130	CD1	C8	3.9	1.1
F183	CE2	N7	3.8	1.1

F183	CZ	N7	3.9	1.1
F183	CE1	N7	4.2	1.2
F183	CD1	N7	4.4	1.3
G193	C	N7	4.4	1.3
G193	C	N7	4.0	1.2
F183	CD2	N7	4.0	1.2
F183	CG	N7	4.3	1.3
V114	CG2	N7	4.1	1.2
V114	CG1	N7	4.2	1.2
L130	CD1	N7	3.7	1.1
L130	CB	N7	4.4	1.3
F183	CE2	C4	4.2	1.2
F183	CZ	C4	3.5	1.0
F183	CE1	C4	3.4	1.0
F183	CD1	C4	4.0	1.1
A80	CB	C4	4.3	1.2
F183	CZ	C6	4.4	1.3
F183	CE1	C6	3.8	1.1
F183	CD1	C6	3.5	1.0
C133	O	C6	4.1	1.2
A80	CB	C6	3.7	1.1
F183	CD2	C6	4.5	1.3
F183	CG	C6	3.9	1.1
V114	CG1	C6	4.4	1.3
C133	CB	C6	4.5	1.3
C133	N	C6	4.1	1.2
E131	O	C6	3.4	1.0
F183	CD1	N6	4.0	1.2
F183	CG	N6	4.0	1.2
V114	CG2	N6	3.8	1.1
V114	CG1	N6	3.4	1.0
V114	CB	N6	4.3	1.3
C133	SG	N6	4.4	1.3
C133	CB	N6	3.7	1.1
C133	CA	N6	4.2	1.3
C133	N	N6	3.8	1.2
E131	O	N6	2.8	0.9
E131	C	N6	4.0	1.2
F183	CE1	N1	3.9	1.1

C133	N	N1	3.4	1.1
E131	O	N1	3.5	1.1
C67	SG	N3	4.5	1.3
F183	CZ	N3	4.1	1.2
F183	CE1	N3	3.5	1.0
F183	CD1	N3	4.1	1.2
F183	CD1	N3	3.9	1.1
L59	CD1	N3	4.1	1.2
D194	OD2	O3	3.9	1.3
D194	CG	O3	3.5	1.1
K82	CD	O3	4.1	1.3
C67	SG	C3	3.8	1.1
D194	OD1	C3	3.6	1.1
D194	CG	C3	4.1	1.2
C67	CB	C3	4.1	1.2
C67	SG	C4A	4.1	1.2
D194	OD1	C4A	4.1	1.2

Table 5. PLK1 contact model (Quanta) for ATP.

PLK1 residue	**Residue atom**	**Protein – ligand atom distance (Å)**
L59	HG	3.5
L59	HD11	3.2
L59	HG	2.6
L59	HD13	3.1
G60	CA	2.8
G60	C	3.2
G60	HA1	1.9
G60	HA2	3.1
G60	HA1	3.5
G60	HA1	3.5
G60	HA1	2.9
K61	N	3.0
K61	H	2.2
G62	HA1	3.1
G63	H	2.9
C67	HG	3.1
C67	HB2	3.0
C67	HG	3.2
C67	HG	3.0
C67	HG	3.4
C67	HB2	3.3
C67	HG	3.2
C67	HG	3.2

C67	HG	2.9
C67	SG	3.0
C67	HG	2.7
C67	CB	2.9
C67	SG	3.3
C67	HB1	2.9
C67	HB2	2.2
C67	HG	2.5
C67	CB	3.3
C67	SG	3.0
C67	HB2	2.6
C67	HG	2.7
A80	CB	3.4
A80	HB1	2.9
A80	HB2	3.1
A80	HB3	3.2
A80	CB	3.3
A80	HB1	3.2
A80	HB2	2.9
A80	HB3	3.1
A80	HB1	3.0
A80	HB1	3.2
A80	HB2	3.0
A80	HB3	3.4
K82	CD	3.3
K82	CE	3.3
K82	NZ	3.4
K82	HZ2	2.8
K82	HB2	3.1
K82	HD1	2.4
K82	HE2	3.0
K82	HD1	3.4
K82	HD1	3.1
K82	HB2	3.5
K82	CE	3.4
K82	NZ	3.1
K82	HZ1	3.5
K82	HZ2	2.2
K82	HE1	2.9

V114	HG13	2.7
V114	HG21	3.4
V114	HG23	3.2
V114	CB	3.3
V114	CG1	2.5
V114	CG2	2.9
V114	HG11	3.4
V114	HG12	2.5
V114	HG13	1.8
V114	HG21	2.8
V114	HG23	2.3
V114	HG12	3.2
V114	HG13	3.2
L130	HD11	3.1
L130	HD11	2.8
L130	HD11	3.0
L130	HB2	3.2
E131	O	3.4
E131	O	2.8
E131	O	3.5
E131	O	3.3
E131	C	3.1
E131	O	2.0
C133	O	3.4
C133	H	3.3
C133	H	2.9
C133	HB1	2.7
C133	N	3.4
C133	O	3.1
C133	H	2.8
C133	O	3.0
C133	HB1	3.4
C133	N	2.9
C133	CB	3.1
C133	H	2.0
C133	HB1	2.3
R135	HH12	3.0
R135	NH1	3.3
R135	HH12	2.7
R135	HH11	2.9
R135	NH1	3.1
R135	HH12	2.9
R135	HH11	2.7
R135	CZ	3.0
R135	NH1	2.3
R135	NH2	3.3

R135	HH12	1.9
R135	HH11	2.1
R135	HH22	2.8
R135	NH1	3.3
R135	HH12	3.0
R135	HH11	3.4
R135	NH1	2.6
R135	HH12	2.3
R135	HH11	3.0
K178	NZ	3.1
K178	HZ1	3.1
K178	HZ2	2.3
F183	HE1	3.3
F183	HZ	2.8
F183	HZ	3.2
F183	CZ	3.5
F183	HZ	3.2
F183	CE1	3.4
F183	HE1	3.3
F183	HD1	3.3
F183	CE1	3.5
F183	HE1	3.0
F183	HZ	3.1
G193	HA2	3.5
G193	HA2	3.1
G193	C	3.4
G193	HA2	3.2
D194	CG	3.2
D194	OD1	3.1
D194	OD2	2.5
D194	OD2	3.4
D194	OD2	3.3
D194	OD2	3.4
D194	OD1	2.6
D194	CB	3.3
D194	CG	2.6
D194	OD1	3.0
D194	OD2	2.7
D194	CB	2.3

D194	OD2	1.6
D194	CG	2.6
D194	OD1	1.7
D194	OD2	3.1

Table 6. PLK1 contact model (Maestro) for 5'-thioadenosine.

PLK1		5'-Thio-adenosine atom	Distance (Å)	Contact cut-off ratio
Residue	*Atom*			
G60	CA	S5	4.0	1.1
C67	N	S5	3.3	1.0
K66	C	S5	3.9	1.1
K66	CA	S5	4.1	1.2
K61	CA	S5	4.3	1.2
K61	N	S5	3.9	1.2
G60	O	S5	3.4	1.0
G60	C	S5	3.5	1.0
C67	SG	S5	3.3	0.9
C67	CB	S5	3.6	1.0
C67	CA	S5	4.1	1.2
R135	NH2	C5A	3.7	1.2
R135	CZ	C5A	4.0	1.2
R135	NH2	C5A	3.6	1.1
C67	SG	C5A	3.6	1.0
C67	CB	C5A	4.2	1.2
F183	CZ	C5	3.5	1.0
F183	CE1	C5	3.5	1.0
F183	CD1	C5	4.1	1.2
A80	CB	C5	3.8	1.1
F183	CE2	C5	4.0	1.2
D194	OD1	O2	3.6	1.2
D194	CG	O2	3.3	1.0
K82	NZ	O2	3.1	1.0
K82	CB	O2	3.8	1.2
K82	CE	O2	3.1	1.0
K82	CD1	O2	3.2	1.0
K82	CG	O2	4.0	1.3
D194	OD2	C2A	3.4	1.0
D194	OD1	C2A	3.6	1.1
D194	CG	C2A	3.8	1.1
K82	CB	C2A	4.1	1.2
C67	CB	C2A	3.9	1.2
K82	CE	C2A	4.2	1.2
K82	CD	C2A	3.9	1.1
F183	CZ	C2	4.2	1.2

C133	O	C2	3.5	1.1
F183	CE1	C2	3.5	1.0
F183	CD1	C2	4.0	1.2
R135	NH2	C2	4.1	1.3
L59	CD1	C2	3.8	1.1
L59	CG	C2	4.2	1.2
A80	CB	C2	3.4	1.0
R135	NH2	O4	3.0	1.0
R135	CZ	O4	3.3	1.0
D194	OD1	O4	3.8	1.3
R135	NH2	O4	2.8	0.9
C67	SG	O4	3.6	1.1
C67	CB	O4	3.9	1.2
F183	CZ	C1	4.2	1.2
R135	NH2	C1	3.7	1.2
R135	CZ	C1	4.3	1.3
D194	OD2	C1	3.6	1.1
D194	OD1	C1	3.3	1.0
D194	CG	C1	3.7	1.1
R135	NH2	C1	3.9	1.2
C67	CB	C1	4.4	1.3
F183	CZ	N9	3.7	1.1
F183	CE1	N9	4.2	1.3
F183	CZ	C8	3.8	1.1
D194	OD2	C8	4.3	1.2
F183	CE2	C8	4.1	1.2
L130	CD1	C8	3.6	1.1
F183	CZ	N7	3.8	1.1
F183	CE1	N7	4.2	1.3
F183	CE2	N7	3.9	1.2
L130	CD1	N7	3.6	1.1
L130	CB	N7	3.9	1.2
F183	CZ	C4	3.5	1.0
F183	CE1	C4	3.6	1.0
R135	NH2	C4	4.1	1.2
A80	CB	C4	4.0	1.2
F183	CE2	C4	4.4	1.3
F183	CZ	C6	3.9	1.1
C133	O	C5	4	1.2

E131	O	C6	3.5	1.1
F183	CE1	N6	4.0	1.2
F183	CD1	N6	3.7	1.1
A80	CB	N6	4.1	1.3
F183	CG	N6	3.9	1.2
C133	SG	N6	4.3	1.3
C133	SB	N6	3.6	1.1
F183	CE1	N6	4.1	1.3
C133	N	N6	3.7	1.2
E131	O	N6	2.9	1.0
V114	CG2	N6	4.1	1.3
V114	CG1	N6	3.7	1.1
F125	CE2	N6	4.0	1.2
F183	CZ	N1	4.3	1.3
C133	O	N1	3.1	1.0
C133	C	N1	3.8	1.2
F183	CE1	N1	3.4	1.0
F183	CD1	N1	3.6	1.1
A80	CB	N1	3.3	1.0
C133	CA	N1	4.1	1.2
C133	N	N1	3.6	1.1
E131	O	N1	3.8	1.2
F183	CZ	N3	4.0	1.2
F183	CE1	N3	3.6	1.1
R135	NH2	N3	3.4	1.1
C67	SG	N3	4.0	1.2
L59	CD1	N3	3.8	1.2
A80	CB	N3	3.8	1.1
D194	OD2	O3	3.0	0.9
D194	CG	O3	3.2	1.0
K82	NZ	O3	3.7	1.2
K82	CE	O3	4.1	1.3
K82	CD	O3	3.5	1.1
D194	OD2	C3	3.7	1.1
D194	OD1	C3	3.3	1.0
D194	CG	C3	3.9	1.2
C67	SG	C3	4.5	1.3
C67	CB	C3	4.1	1.2
K82	CD	C3	3.8	1.1
R135	NH2	C4A	3.4	1.0
R135	CZ	C4A	3.9	1.1
D194	OD2	C4A	4.4	1.3
D194	OD1	C4A	3.3	1.0
D194	CG	C4A	4.2	1.2
R135	NH2	C4A	3.6	1.1
C67	SG	C4A	4.0	1.1

C67	CB	C4A	4.2	1.2

Table 7. PLK1 contact model (Quanta) for 5'-thioadenosine.

PLK1 residue	Residue atom	Protein – ligand atom distance (Å)
L59	HG	3.4
L59	HD11	3.5
L59	HD13	3.3
L59	HD11	3.2
L59	CG	3.2
L59	CD1	3.0
L59	HG	2.5
L59	HD11	2.9
L59	HD13	2.5
G60	C	3.2
G60	O	3.2
G60	HA1	3.1
G60	HA1	3.3
C67	N	3.1
C67	CB	3.1
C67	SG	2.0
C67	H	2.7
C67	HB2	3.0
C67	SG	3.2
C67	HB2	3.0
C67	SG	3.4
C67	HB2	3.4
C67	HB2	3.1
C67	SG	3.4
C67	CB	3.1
C67	HB1	3.2
C67	HB2	2.1
C67	CB	3.5
C67	HB2	2.6
A80	HD1	3.4
A80	HE3	3.2

A80	HB3	3.4
A80	CB	3.3
A80	HB1	3.1
A80	HB2	2.9
A80	HB3	3.2
A80	HB1	2.9
A80	HB1	3.3
A80	HB2	3.3
K82	CD	3.2
K82	CE	3.1
K82	NZ	3.1
K82	HZ2	2.5
K82	HB2	3.0
K82	HD1	2.5
K82	HE2	2.6
K82	HB2	3.1
K82	HD1	2.9
K82	HZ2	3.1
K82	HD1	2.5
K82	HD1	2.7
K82	CB	3.5
K82	HB2	2.4
K82	HD1	3.1
K82	CE	3.3
K82	NZ	2.9
K82	HZ2	2.0
K82	HD1	2.9
K82	HE2	3.1
K82	HZ2	2.9
K82	HD1	3.2
K82	HB2	3.3
K82	HD1	2.6
V114	HG13	3.3
V114	HG13	2.9
V114	HG23	3.5
V114	CG1	2.8
V114	CG2	3.3
V114	HG12	2.8
V114	HG13	1.9
V114	HG21	3.2
V114	HG23	2.7
V114	HG13	3.5
L130	HD13	3.2
L130	HD11	3.0
L130	HB1	3.4
L130	HB2	3.4

L130	HD13	3.5
L130	HD11	2.8
L130	CD1	3.2
L130	HD13	2.9
L130	HD11	2.6
L130	HB2	3.2
E131	O	3.5
E131	O	2.9
E131	O	3.2
E131	O	2.5
C133	H	3.2
C133	H	2.9
C133	HB1	2.7
C133	O	3.1
C133	H	2.7
C133	O	3.1
C133	HB1	3.2
C133	N	2.7
C133	CA	3.2
C133	CB	2.8
C133	SG	3.4
C133	H	2.0
C133	HB1	2.0
R135	HH11	3.1
R135	HH22	3.2
R135	CZ	3.3
R135	NH1	2.8
R135	NH2	3.0
R135	HH11	1.8
R135	HH22	2.1
R135	HH11	3.0
R135	HH22	2.7
R135	HH11	3.4
R135	HH11	3.3
R135	NH1	3.4
R135	HH11	2.8
R135	NH2	3.4
R135	HH11	2.8
R135	[illegible]	2.5

R135	HH11	3.4
R135	HH22	2.5
R135	NH2	2.9
R135	HH11	3.2
R135	HH21	3.5
R135	HH22	2.1
F183	CE1	3.5
F183	HE1	2.9
F183	HZ	3.3
F183	HZ	3.1
F183	HZ	3.5
F183	HE1	3.4
F183	HZ	3.2
F183	CE1	3.4
F183	CE1	3.4
F183	HD1	3.4
F183	HE1	3.2
F183	HE1	2.9
F183	HE1	3.2
F183	HZ	2.9
D194	CG	3.3
D194	OD2	2.5
D194	OD2	3.4
D194	OD1	3.3
D194	CG	3.2
D194	OD1	2.6
D194	OD2	3.0
D194	OD1	3.3
D194	OD1	3.3
D194	CG	2.7
D194	OD1	2.4
D194	OD2	2.9
D194	OD2	3.4
D194	H	3.3
D194	CG	2.4
D194	OD1	2.8
D194	OD2	1.5
D194	CG	2.3
D194	OD1	1.7
D194	OD2	2.3
D194	OD1	2.4

Table 8. PLK1 contact model (Maestro) for staurosporine.

PLK1		Staurosporine atom	Distance (Å)	Contact cut-off ratio
Residue	*Atom*			
C67	CB	O4	3.5	1.1
D194	OD2	C21	4.1	1.2
C67	CB	C23	4.2	1.2
C67	SG	C18	3.7	1.0
C67	CB	C18	3.9	1.1
C67	SG	C19	4.3	1.2
C67	CB	C19	4.2	1.2
D194	OD1	C16	3.4	1.0
D194	CG	C16	4.0	1.2
G193	O	C16	3.7	1.1
G193	C	C16	4.3	1.3
L130	CD1	C16	4.3	1.3
F183	CE1	C14	3.3	1.0
F183	CZ	C14	3.7	1.1
F183	CD1	C14	4.1	1.2
L130	CD2	C14	4.3	1.3
L130	CD1	C14	3.9	1.1
L130	CG	C14	4.2	1.2
L130	CB	C14	3.8	1.1
A80	CB	C14	4.2	1.2
D194	OD1	C15	3.9	1.2
G193	O	C15	3.6	1.1
G193	C	C15	4.1	1.2
F183	CE1	C15	3.8	1.1
L130	CD2	C15	3.9	1.2
L130	CD1	C15	3.6	1.1
L130	CG	C15	4.1	1.2
L130	CB	C15	4.3	1.2
F183	CE1	C13	3.8	1.1
F183	CZ	C13	4.3	1.2
F183	CD1	C13	4.2	1.2
C67	SG	C13	4.6	1.3
A80	CB	C13	3.4	1.0
C67	SG	C12	3.3	1.1

L59	CB	C7	3.8	1.1
C67	SG	C10	4.1	1.2
A80	CB	C10	4.3	1.3
L59	CD1	C10	3.9	1.1
C67	SG	C11	3.6	1.0
C67	CB	C11	4.4	1.3
A80	CB	C11	4.4	1.3
R135	CG	C6	4.0	1.2
L59	C	C6	4.4	1.3
L59	CB	C6	3.8	1.1
G60	CA	N3	4.2	1.3
G60	CA	C20	3.8	1.1
G60	N	C20	4.2	1.3
L59	C	C20	4.3	1.2
L59	O	C20	4.1	1.3
R135	CG	C5	3.7	1.1
G60	CA	C5	4.3	1.3
G60	N	C5	4.2	1.3
L59	C	C5	3.9	1.1
L59	CB	C5	4.1	1.2
L59	O	C5	3.7	1.1
R135	CG	C4	3.5	1.0
R135	NE	C4	3.7	1.1
R135	CD	C4	4.0	1.2
L59	C	C4	3.8	1.1
L59	CB	C4	4.4	1.3
L59	O	C4	3.2	1.0
R135	CG	C3	4.1	1.2
R135	CD	C3	4.4	1.3
L59	C	C3	4.1	1.2
L59	O	C3	3.2	1.0
G60	CA	C2	4.1	1.2
L59	O	C2	3.8	1.2
G60	CA	C1	3.7	1.1
L59	O	C1	4.2	1.3
C67	CB	C25	4.4	1.3
G60	CA	C25	4.3	1.3
D194	OD2	C23	4.0	1.2
D194	CG	C22	4.0	1.2
D194	OD2	C22	3.5	1.0
D194	OD1	C26	3.9	1.2
D194	CG	C26	4.0	1.2
D194	OD2	C26	3.4	1.0
K82	CE	C26	4.2	1.2
K82	CD	C26	3.9	1.1
K82	CG	C26	4.4	1.3

C67	CB	C26	4.2	1.2
G180	O	O6	3.7	1.2
N181	O	C27	3.8	1.2
N181	C	C27	4.2	1.2
N181	CA	C27	3.8	1.1
G180	O	C27	3.6	1.1
G180	C	C27	4.2	1.2
D194	CG	C27	4.4	1.3
D194	N	C27	3.9	1.2
G193	O	C27	3.1	1.0
G193	C	C27	4.0	1.2
G180	O	N4	3.6	1.2
D194	OD2	N4	4.2	1.3
N181	OD1	C28	4.1	1.3
K178	NZ	C28	3.7	1.1
D176	OD2	C28	4.4	1.3
D194	CG	C28	4.1	1.2
D194	CB	C28	4.1	1.2
D194	OD2	C28	3.3	1.0
C133	O	C9	3.5	1.1
C133	C	C9	3.8	1.1
C133	N	C9	3.9	1.2
A80	CB	C9	3.9	1.2
L59	CD1	C9	3.9	1.1
R134	CA	N1	4.0	1.2
R134	N	N1	4.0	1.3
C133	O	N1	2.8	0.9
C133	C	N1	3.4	1.0
L59	CD2	N1	4.2	1.3
L59	CD1	N1	3.8	1.2
R135	CG	O5	3.8	1.2
R135	NH2	O5	3.1	1.0
R135	CZ	O5	3.4	1.1
R135	CD	O5	3.8	1.2
L59	CD2	O5	3.6	1.1
L59	CG	O5	4.1	1.3
L59	CB	O5	3.9	1.2
R135	CG	C8	3.9	1.1
C133	O	C8	3.8	1.2

Table 9. PLK1 contact model (Quanta) for staurosporine.

PLK1 residue	Residue atom	Protein – ligand atom distance (Å)
L59	HB1	2.8
L59	HD13	3.1
L59	HD13	3.0
L59	HB1	2.9
L59	HB1	3.2
L59	O	3.2
L59	HB1	3.4
L59	O	3.2
L59	HD13	2.8
L59	HD13	2.7
L59	HD22	3.3
L59	HB1	3.0
L59	HD22	2.6
L59	HB1	2.9
L59	HD13	2.9
L59	HD22	2.9
L59	O	3.4
L59	HB1	3.1
L59	O	3.5
L59	CD1	3.3
L59	HD13	2.4
L59	HD13	3.1
L59	HD22	3.2
G60	HA1	3.2
G60	HA1	2.8
G60	HA1	3.5
G60	HA1	3.3
G60	HA1	2.7
G60	HA1	3.3
G60	HA1	2.9
G60	CA	3.4
G60	C	3.4
G60	HA1	2.5
C67	HB1	2.8
C67	HB2	3.3
C67	HB1	3.3
C67	HB1	3.4
C67	HB1	3.1
C67	HB1	3.5
C67	CB	3.4

C67	HB1	2.3
C67	HG	3.5
A80	HB2	3.5
A80	CB	3.4
A80	HB2	3.0
A80	HB3	2.9
A80	HB3	3.1
A80	HB3	3.4
A80	HB1	3.3
A80	HB2	3.4
A80	CB	3.0
A80	HB1	3.0
A80	HB2	2.6
A80	HB3	2.7
A80	CB	2.9
A80	HB1	2.2
A80	HB2	3.3
A80	HB3	2.7
K82	HD2	3.0
K82	HD2	3.4
K82	HD2	3.3
K82	HE1	3.1
K82	CD	3.5
K82	HZ3	2.9
K82	HD2	2.5
K82	HE1	3.3
K82	HB2	3.1
K82	HG1	3.3
K82	HD2	2.7
L130	HD12	3.3
L130	HB1	3.0
L130	HD12	2.9
L130	HD22	3.5
L130	HD12	2.6
L130	HD22	3.1
L130	CD1	3.4
L130	CD2	3.1
L130	HD12	2.6
L130	HD22	

L132	HA	3.5
L132	C	3.4
C133	O	2.8
C133	C	3.4
C133	O	3.5
C133	H	3.4
C133	HB1	3.1
C133	N	3.5
C133	H	3.4
C133	C	2.7
C133	O	1.8
C133	O	1.8
R134	HA	3.1
R134	HA	3.4
R134	HA	3.4
R134	HA	2.8
R135	HG2	3.0
R135	HG2	3.3
R135	HG1	3.0
R135	HG2	3.3
R135	CG	3.5
R135	HE	3.2
R135	HG1	2.7
R135	HG2	3.3
R135	HG1	3.1
R135	HE	3.4
R135	NE	2.8
R135	CZ	3.4
R135	NH2	3.1
R135	HE	1.7
R135	HG2	3.0
R135	HH21	2.2
R135	HE	2.6
R135	HG2	2.9
R135	HH21	3.4
R135	CG	3.5
R135	NE	3.0
R135	HE	2.4
R135	HG1	3.0
R135	HG2	3.2
R135	HH21	3.2
R135	H	3.3
R135	HE	3.5
R135	HE	1.7
K178	HZ1	3.5
K178	HZ1	2.7

K178	HZ1	3.2
K178	NZ	3.5
K178	HZ1	2.5
K178	NZ	2.9
K178	HZ1	2.0
K178	HZ2	3.2
K178	HZ3	3.5
K178	HZ1	2.0
G180	O	3.5
G180	O	3.3
G180	O	2.6
N181	HA	2.8
N181	CA	3.4
N181	OD1	3.2
N181	HA	2.3
N181	CA	3.2
N181	C	3.5
N181	O	3.2
N181	HA	2.3
N181	OD1	3.2
F183	CE1	3.3
F183	HE1	2.8
F183	HE1	2.9
F183	HE1	2.9
F183	CE1	3.0
F183	CZ	3.0
F183	HE1	2.6
F183	HZ	2.7
G193	O	3.1
G193	HA2	3.4
G193	O	3.0
G193	O	3.3
G193	O	2.5
D194	OD1	3.4
D194	OD2	3.4
D194	H	3.0
D194	OD2	3.3
D194	HB2	3.3
D194	CG	3.0

D194	CG	3.0
D194	OD1	2.8
D194	OD2	2.6
D194	N	3.2
D194	H	2.2
D194	HB2	2.8
D194	H	3.5
D194	H	3.0
D194	OD2	2.7
D194	CB	3.2
D194	CG	3.3
D194	OD2	2.9
D194	HB1	3.5
D194	HB2	2.3
D194	H	2.2

Table 10. PLK1 contact model (Maestro) for 4-[4-(4-methyl-2-methylamino-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol.

PLK1		**Ligand atom**	**Distance (Å)**	**Contact cut-off ratio**
Residue	*Atom*			
D194	OD2	NM1	3.8	1.2
K82	CD	NM1	4.1	1.3
D194	CG	CM12	4.0	1.2
D194	OD2	CM12	3.6	1.1
F64	CG	CM12	4.0	1.2
D194	OD1	CM12	3.5	1.1
K82	NZ	CM12	4.2	1.3
K82	CD	CM12	3.9	1.1
F64	CD1	CM12	4.1	1.2
F64	CB	CM12	3.8	1.1
D194	CG	C	4.0	1.2
D194	OD2	C	3.5	1.0
D194	OD1	C	3.8	1.2
K82	CD	C	4.1	1.2
C67	CB	C	4.0	1.2
D194	CG	N	3.5	1.1
D194	OD2	N	3.4	1.0
D194	OD1	N	3.1	1.0
K82	NZ	N	3.4	1.1
K82	CE	N	3.4	1.0
K82	CD	N	3.5	1.1
K82	CB	N	4.2	1.3
D194	CG	C1	3.9	1.1

D194	OD2	C1	3.8	1.1
D194	OD1	C1	3.7	1.2
K82	NZ	C1	4.1	1.2
K82	CE	C1	4.1	1.2
L130	CD1	C1	4.1	1.2
D194	CG	CM2	3.7	1.1
D194	CB	CM2	4.3	1.3
D194	CA	CM2	4.1	1.2
D194	OD2	CM2	4.0	1.2
D194	NZ	CM2	3.6	1.1
D194	OD1	CM2	3.5	1.1
K82	NZ	CM2	3.9	1.2
K82	CE	CM2	4.1	1.2
L130	CD2	CM2	3.9	1.2
L130	CD1	CM2	3.8	1.1
D194	OD2	S	4.2	1.2
C67	SG	S	3.5	1.0
C67	CB	S	3.3	0.9
D194	OD2	C2	4.3	1.3
F183	CZ	C2	4.1	1.2
C67	SG	C2	3.9	1.1
C67	CB	C2	4.3	1.3
F183	CZ	N1	4.0	1.2
F183	CG	N1	4.2	1.3
F183	CE1	N1	3.5	1.1
F183	CD1	N1	3.6	1.1
C133	N	N1	3.8	1.2
E131	O	N1	3.6	1.2
A80	CB	N1	3.3	1.0
C133	O	N1	3.4	1.1
C133	C	N1	4.2	1.3
F183	CD2	C3	4.3	1.3
F183	CE2	C3	4.2	1.2
F183	CZ	C3	4.0	1.2
F183	CG	C3	4.3	1.3
F183	CE1	C3	4.0	1.2
F183	CD1	C3	4.1	1.2
E131	O	C3	3.5	1.1
A80	CB	C3	3.5	1.0

F183	CZ	C5	3.6	1.0
F183	CE1	C5	4.0	1.2
C67	SG	C5	3.9	1.1
A80	CB	C5	4.1	1.2
F183	CZ	N6	3.6	1.1
F183	CE1	N6	3.5	1.1
C67	SG	N6	3.5	1.0
A80	CB	N6	3.9	1.2
F183	CZ	C7	3.8	1.1
F183	CE1	C7	3.3	1.0
F183	CD1	C7	3.8	1.1
C67	SG	C7	4.2	1.2
A80	CB	C7	3.5	1.0
C133	O	C7	3.6	1.1
F183	CE1	N2	3.4	1.0
F183	CD1	N2	3.8	1.2
A80	CB	N2	4.2	1.3
C133	O	N2	2.8	0.9
C133	C	N2	4.0	1.2
L59	CD2	N2	3.9	1.2
F183	CE1	C8	3.9	1.1
C133	O	C8	3.6	1.1
L59	CD2	C8	3.8	1.1
L59	CG	C8	4.2	1.2
L59	CB	C8	4.1	1.2
R135	CB	C9	4.4	1.3
R135	N	C9	4.1	1.3
R134	CA	C9	4.2	1.2
C133	O	C9	3.4	1.0
C133	C	C9	4.4	1.3
L59	CD2	C9	3.9	1.1
L59	CG	C9	4.0	1.2
L59	CB	C9	4.3	1.2
R135	NH2	O11	2.9	1.0
R135	NH1	O11	3.4	1.1
R135	CZ	O11	3.5	1.1
L59	C	O11	3.5	1.1
R135	NH2	C10	4.1	1.3
R135	CZ	C10	4.4	1.3
L59	CG	C10	4.1	1.2
L59	CB	C10	4.2	1.2
R135	NH2	C11	3.4	1.1
R135	NH1	C11	3.5	1.1
R135	CZ	C11	3.6	1.1
L59	C	C11	3.7	1.1
L59	CG	C11	4.4	1.3

L59	CB	C11	4.0	1.2
L59	O	C11	3.2	1.0
L59	CA	C11	4.3	1.2
R135	NH1	C12	4.2	1.3
F183	CE1	C12	4.3	1.2
C67	SG	C12	4.3	1.2
L59	C	C12	4.4	1.3
L59	CD2	C12	4.4	1.3
L59	CG	C12	4.4	1.3
L59	CB	C12	3.8	1.1
R135	NH2	C13	4.0	1.2
R135	NH1	C13	3.3	1.0
R135	CZ	C13	3.8	1.1
G60	CA	C13	4.3	1.2
G60	N	C13	3.8	1.2
L59	C	C13	3.5	1.0
L59	CB	C13	3.8	1.1
L59	O	C13	3.4	1.1
L59	CA	C13	4.2	1.2

Table 11. PLK1 contact model (Quanta) for 4-[4-(4-methyl-2-methylamino-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol.

PLK1 residue	Residue atom	Protein – ligand atom distance (Å)
L59	O	1.7
L59	HD23	2.9
L59	HB1	3.1
L59	HD23	2.9
L59	HB1	3.5
L59	HG	3.3
L59	HD23	3.2
L59	O	2.7
L59	HG	3.3
L59	O	3.2
L59	HB1	3.2
L59	HB1	3.7

L59	HA	3.4
L59	HB1	3.1
L59	C	3.2
L59	O	3.2
L59	HB1	3.1
G60	N	3.2
G60	CA	3.4
G60	HA1	2.6
F64	HB2	2.9
F64	HB2	3.5
F64	CB	3.4
F64	HB2	2.4
F64	HD1	3.2
F64	CB	3.2
F64	HB1	3.0
F64	HB2	2.5
C67	HB1	3.3
C67	HB1	3.0
C67	CB	3.3
C67	HB1	2.6
C67	HB2	3.4
C67	SG	3.5
C67	HB1	3.0
C67	HB2	3.3
A80	CB	3.3
A80	HB1	3.0
A80	HB2	3.1
A80	HB3	3.0
A80	CB	3.5
A80	HB1	3.3
A80	HB3	2.9
A80	HB1	3.4
A80	HB3	3.4
A80	HB1	3.3
A80	HB1	3.0
A80	HB1	2.9
A80	HB2	3.4
A80	HB3	3.0
K82	HD1	3.0
K82	HD1	2.9
K82	HD1	3.1
K82	CD	3.5
K82	CE	3.4
K82	NZ	3.4
K82	HZ2	2.7
K82	HB2	3.4

K82	HD1	2.7
K82	HE2	3.0
K82	HE2	3.3
K82	HZ2	3.4
K82	HE2	3.3
K82	HZ2	3.0
K82	HD1	3.4
K82	CD	3.0
K82	HZ2	3.2
K82	HD1	2.2
K82	HD2	2.9
K82	HE2	3.0
K82	NZ	3.1
K82	HZ2	2.6
K82	HZ3	2.9
K82	HE2	3.1
V114	HG12	2.9
V114	HG12	3.5
L130	HD13	3.3
L130	HD13	3.1
L130	HD22	3.2
L130	HB1	3.5
L130	HB1	3.3
L130	HD13	3.0
L130	HD22	3.1
L130	CG	3.4
L130	CD1	2.8
L130	CD2	2.9
L130	HD13	2.3
L130	HD11	2.6
L130	HD22	2.3
L130	HD21	2.8
L130	HB1	3.1
L130	CD1	3.3
L130	HB1	2.8
L130	HD13	2.4
L130	HD22	2.8
E131	O	3.5
E131	O	2.0

C133	O	1.8
C133	O	2.6
R134	HA	3.2
R134	CA	3.3
R134	HA	2.3
R135	HH22	2.0
R135	H	3.2
R135	HB1	3.4
R135	CZ	3.5
R135	NH1	3.4
R135	NH2	2.9
R135	HH11	2.8
R135	HH22	2.0
R135	H	3.5
R135	NH2	3.4
R135	HH11	3.1
R135	HH22	2.8
R135	NH1	3.3
R135	HH11	2.9
R135	H	2.9
R135	H	3.5
R135	HH11	3.3
R135	HH22	2.8
R135	NH1	2.9
R135	HH12	3.2
R135	HH11	2.4
F183	HZ	3.5
F183	HZ	3.3
F183	HE1	3.2
F183	HZ	3.4
F183	CE1	3.3
F183	HE1	3.0
F183	CE1	3.4
F183	HE1	2.8
F183	HE1	2.9
F183	HE1	3.3
F183	HE2	3.1
F183	HD1	3.3
F183	HE1	3.2
F183	HE1	3.4
G193	HA2	3.3
D194	OD2	3.5
D194	OD1	3.1
D194	OD2	3.4
D194	H	3.2
D194	CG	2.9

D194	OD1	2.5
D194	OD2	2.6
D194	N	3.0
D194	H	2.7
D194	H	3.4
D194	N	3.1
D194	CA	3.3
D194	CG	3.0
D194	OD1	2.6
D194	H	2.7
D194	HA	2.7

CLAIMS

1. A method of screening for a modulator of PLK, wherein the method comprises using the structure co-ordinates of Table 2.

2. A method according to claim 1 comprising the steps of:

(a) providing at least a portion of the structure co-ordinates of Table 2;

(b) employing at least a portion of the structure co-ordinates of Table 2 to design or select or synthesise a putative modulator of PLK;

(c) contacting the putative modulator of PLK with PLK or a mutant, variant, homologue, derivative or fragment thereof, in the presence of a substrate of PLK; and

(d) determining whether said putative modulator of PLK modulates PLK.

3. A method according to claim 1 or claim 2 wherein at least a portion of the structure co-ordinates of Table 2 and/or the putative modulator of PLK and/or the substrate are provided on a machine-readable data storage medium comprising a data storage material encoded with machine readable data.

4. A method according to claim 2 or claim 3 wherein the putative modulator of PLK is selected from a library of compounds.

5. A method according claim 2 or claim 3 wherein the putative modulator of PLK is selected from a database.

6. A method according to claim 2 or claim 3 wherein the putative modulator of PLK is designed *de novo*.

7. A method according to claim 2 or claim 3 wherein the putative modulator of PLK is designed from a known PLK modulator.

8. A method according to claim 2 or claim 3 wherein the design or selection of the putative modulator of PLK is performed in conjunction with computer modelling.

9. A method according to any preceding claim wherein the putative modulator of PLK inhibits PLK activity.

10. A method according to any preceding claim wherein the PLK is PLK1.

11. A method according to any preceding claim wherein the putative modulator of PLK is useful in the prevention and/or treatment of a PLK related disorder.

12. A method according to claim 11 wherein the PLK related disorder is a proliferative disorder.

13. A method according to claim 12 wherein the proliferative disorder is selected from cancer, leukemia, glomerulonephritis, rheumatoid arthritis, psoriasis and chronic obstructive pulmonary disorder.

14. An assay for a candidate compound capable of modulating PLK, said assay comprising the steps of:

(a) contacting said candidate compound with PLK;

(b) detecting whether said candidate compound forms associations with one or more amino acid residues corresponding to PLK amino acid residues L59, G60, C67, A80, K82, L130, C133, R135, F183 and D194.

15. An assay according to claim 14 wherein said candidate compound is selected by performing rational drug design with a 3-dimensional model of PLK in conjunction with computer modelling.

(i) 5'-thioadenosine, or a derivative thereof;

(ii) staurosporine, or a derivative thereof; and

(iii) 4-[4-(4-methyl-2-methylaminothiazol-5-yl)-pyrimidin-2-ylamino]-phenol; 4-[4-(2,4-dimethyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol or 4-[4-(2-amino-4-methyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol;

or a pharmaceutically acceptable salt thereof, in an assay for identifying candidate compounds capable of modulating PLK.

18. Use according to claim 17 wherein the assay is a competitive binding assay.

19. Use according to claim 17 or claim 18 wherein the assay comprises contacting a candidate compound with PLK in the presence of a compound selected from:

(i) 5'-thioadenosine, or a derivative thereof;

(ii) staurosporine, or a derivative thereof; and

(iii) 4-[4-(4-methyl-2-methylaminothiazol-5-yl)-pyrimidin-2-ylamino]-phenol, 4-[4-(2,4-dimethyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol or 4-[4-(2-amino-4-methyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol;

or a pharmaceutically acceptable salt thereof, and detecting any change in the interaction between (i), (ii) or (iii) and PLK.

20. A PLK modulator identified by the method of any one of claims 1 to 13, or a candidate compound identified by an assay according to any one of claims 14 to 19.

21. A PLK modulator or candidate compound according to claim 20 wherein the PLK modulator inhibits PLK activity.

22. A PLK modulator or candidate compound according to claim 20 or claim 21 which is capable of forming a covalent bond with the amino acid residue corresponding to PLK amino acid residue C67.

23. A PLK modulator or candidate compound according to claim 22 which is capable of forming a disulfide bond with the thiol group of the amino acid residue corresponding to PLK amino acid residue C67.

24. A PLK modulator or candidate compound according to claim 20 which is an irreversible antagonist.

25. A pharmaceutical composition comprising a PLK modulator or candidate compound according to any one of claims 20 to 24 and a pharmaceutically acceptable carrier, diluent, excipient or adjuvant or any combination thereof.

26. A method of preventing and/or treating a PLK related disorder comprising administering a PLK modulator or candidate compound according to any one of claims 20 to 24 and/or a pharmaceutical composition according to claim 25 wherein said PLK modulator, said candidate compound or said pharmaceutical, is capable of causing a beneficial preventative and/or therapeutic effect.

27. A method according to claim 26 wherein the PLK modulator or candidate compound is selected from the following:

(i) 5'-thioadenosine, or a derivative thereof;

(ii) staurosporine, or a derivative thereof; and

(iii) 4-[4-(4-methyl-2-methylaminothiazol-5-yl)-pyrimidin-2-ylamino]-phenol, 4-[4-(2,4-dimethyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol or 4-[4-(2-amino-4-methyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol;

or a pharmaceutically acceptable salt thereof.

28. Use of a PLK modulator according to any one of claims 20 to 24 in the preparation of a

30. A process comprising the steps of:

(a) performing the method according to any of claims 1 to 13, or an assay according to any one of claims 14 to 19;

(b) identifying one or more modulators of PLK; and

(d) preparing a quantity of said one or more PLK modulators.

31. A process comprising the steps of:

(a) performing the method according to any of claims 1 to 13, or an assay according to any one of claims 14 to 19;

(b) identifying one or more PLK modulators; and

(c) preparing a pharmaceutical composition comprising said one or more identified PLK modulators.

32. A process comprising the steps of:

(a) performing the method according to any of claims 1 to 13, or an assay according to any one of claims 14 to 19;

(b) identifying one or more PLK modulators;

(c) modifying said one or more PLK modulators; and

(d) optionally preparing a pharmaceutical composition comprising said one or more PLK modulators.

33. A computer for producing a three-dimensional representation of PLK wherein said computer comprises:

(a) a computer-readable data storage medium comprising a data storage material encoded with computer-readable data, wherein said data comprises the structure co-ordinates of Table 2;

(b) a working memory for storing instructions for processing said computer-readable data;

(c) a central-processing unit coupled to said working memory and to said computer-readable data storage medium for processing said computer-machine readable data into said three-dimensional representation; and

(d) a display coupled to said central-processing unit for displaying said three-dimensional representation.

34. A machine-readable data storage medium comprising a data storage material encoded with machine readable data, wherein the data is defined by at least a portion of the structure co-ordinates of Table 2.

35. Use of the computer of claim 33 or the machine readable data storage medium of claim 34 to predict the structure and/or function of potential modulators of PLK.

36. Use of at least a portion of the structure co-ordinates of Table 2 to screen for modulators of PLK.

37. Use of at least a portion of the structure co-ordinates of Table 2 to solve the structure of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of PLK.

38. Use according to claim 37 wherein the structure of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of PLK is solved using molecular replacement.

39. Use of at least a portion of the structure co-ordinates of Table 2 in molecular design techniques to design, select and synthesise modulators of PLK.

40. Use of at least a portion of the structure co-ordinates of Table 2 in the development of compounds that can isomerise to reaction intermediates in the chemical reaction of a substrate or other compound that binds to PLK.

42. A method of treating a proliferative disorder, said method comprising administering to a subject in need thereof a compound selected from the following:

(i) 5'-thioadenosine, or a derivative thereof;

(ii) staurosporine, or a derivative thereof; and

(iii) 4-[4-(4-methyl-2-methylaminothiazol-5-yl)-pyrimidin-2-ylamino]-phenol, 4-[4-(2,4-dimethylthiazol-5-yl)-pyrimidin-2-ylamino]-phenol or 4-[4-(2-amino-4-methyl thiazol-5-yl)-pyrimidin-2-ylamino]-phenol;

or a pharmaceutically acceptable salt thereof, in an amount sufficient to inhibit PLK such that said proliferative disorder is treated.

43. A method of treating a proliferative disorder comprising inhibiting PLK by administering to a subject in need thereof, a therapeutically effective amount of a compound selected from the following:

(i) 5'-thioadenosine, or a derivative thereof;

(ii) staurosporine, or a derivative thereof; and

(iii) 4-[4-(4-methyl-2-methylaminothiazol-5-yl)-pyrimidin-2-ylamino]-phenol, 4-[4-(2,4-dimethyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol or 4-[4-(2-amino-4-methyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol;

or a pharmaceutically acceptable salt thereof, such that treatment of the proliferative disorder occurs.

44. A method of treating a PLK dependent disorder in a subject in need thereof, said method comprising administering to said subject a compound selected from the following:

(i) 5'-thioadenosine, or a derivative thereof;

(ii) staurosporine, or a derivative thereof; and

(iii) 4-[4-(4-methyl-2-methylaminothiazol-5-yl)-pyrimidin-2-ylamino]-phenol, 4-[4-(2,4-dimethyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol or 4-[4-(2-amino-4-methyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol;

or a pharmaceutically acceptable salt thereof, in an amount sufficient to inhibit PLK.

45. A method according to claim 45 wherein the PLK dependent disorder is a disorder associated with increased PLK activity.

46. A method according to claim 44 or claim 45 wherein the disorder is cancer.

47. A method of inhibiting PLK in a cell comprising contacting said cell with an amount of a compound selected from the following:

(i) 5'-thioadenosine, or a derivative thereof;

(ii) staurosporine, or a derivative thereof; and

(iii) 4-[4-(4-methyl-2-methylaminothiazol-5-yl)-pyrimidin-2-ylamino]-phenol, 4-[4-(2,4-dimethyl-thiazol-5-yl)-pyrimidin-2-ylamino]-phenol or 4-[4-(2-amino-4-methyl thiazol-5-yl)-pyrimidin-2-ylamino]-phenol;

or a pharmaceutically acceptable salt thereof, such that PLK is inhibited in said cell.

48. A method according to claim 47 wherein the cell is a cancer cell.

49. A fragment of PLK, or a homologue, mutant, or derivative thereof, comprising a ligand binding domain, said ligand binding domain being defined by the amino acid residue structural coordinates selected from one or more of the following: L59, G60, C67, A80, K82, L130, C133, R135, F183 and D194.

50. A fragment of PLK, or a homologue, mutant or derivative thereof, according to claim 49 which corresponds to a portion of the structure co-ordinates of Table 2.

51. Use of a fragment of PLK, or a homologue, mutant, or derivative thereof, according to claim 50 or 51 in an assay for identifying candidate compounds capable of modulating PLK.

53. An assay substantially as described herein, and with reference to the accompanying drawings.

54. A PLK modulator substantially as described herein, and with reference to the accompanying drawings.

55. A process substantially as described herein, and with reference to the accompanying drawings.

ABSTRACT

METHOD

The present invention relates to a homology model for PLK, and the use thereof in assays for the indentification of small molecule PLK modulators.

The invention further relates to PLK modulators identified by said assays, and their use in the treatment of PLK-related disorders such as proliferative disorders.

```
sp|P53350|  ----------------MS-AAVTAGKLARA-----PADPGKAGVPGVAAPG---APAAAP
sp|Q9NYY3|  MELLRTITYQPAASTKMCEQALGKGCGADSKKKRPPQPPEESQPPQSQAQVPPAAPHHHH
sp|Q9H4B4|  --------MEPAAG-FLSPRPFQRTAAATA----PPAGPG---PPPSALRGPELEMLAGL
                        :.  ..     * :     *  *     *

sp|P53350|  PAKEIP----EVLVDPRSRRRYVRGRFLGKGGFAKCFEISDADTKEVFAGKIVPKSLLLK
sp|Q9NYY3|  HHSHSGPEISRIIVDPTTGKRYCRGKVLGKGGFAKCYEMTDLTNNKVYAAKIIPHSRVAK
sp|Q9H4B4|  PTSDPG----RLITDPRSGRTYLKGRLLGKGGFARCYEATDTETGSAYAVKVIPQSRVVK
              ..       .::.** : : * :*:.*******:*:* :*  . ..:* *::*:* : *

sp|P53350|  PHQREKMSMEISIHRSLAHQHVVGFHGFFEDNDFVFVVLELCRRRSLLELHKRRKALTEP
sp|Q9NYY3|  PHQREKIDKEIELHRILHHKHVVQFYHYFEDKENIYILLEYCSRRSMAHILKARKVLTEP
sp|Q9H4B4|  PHQREKILNEIELHRDLQHRHIVRFSHHFEDADNIYIFLELCSRKSLAHIWKARHTLLEP
            ******:  **.:** * *:*:* *  .*** : ::::.** * *:*: .: * *:.* **

sp|P53350|  EARYYLRQIVLGCQYLHRNRVIHRDLKLGNLFLNEDLEVKIGDFGLATKVEYDGERKKTL
sp|Q9NYY3|  EVRYYLRQIVSGLKYLHEQEILHRDLKLGNFFINEAMELKVGDFGLAARLEPLEHRRRTI
sp|Q9H4B4|  EVRYYLRQILSGLKYLHQRGILHRDLKLGNFFITENMELKVGDFGLAARLEPPEQRKKTI
            *.*******: * :***.. ::********:*:.* :*:*:******:::*   .*::*:

sp|P53350|  CGTPNYIAPEVLSKKGHSFEVDVWSIGCIMYTLLVGKPPFETSCLKETYLRIKKNEYSIP
sp|Q9NYY3|  CGTPNYLSPEVLNKQGHGCESDIWALGCVMYTMLLGRPPFETTNLKETYRCIREARYTMP
sp|Q9H4B4|  CGTPNYVAPEVLLRQGHGPEADVWSLGCVMYTLLCGSPPFETADLKETYRCIKQVHYTLP
            ******::**** ::**. * *:*::**:***:* * *****: *****  *:: .*::*

sp|P53350|  KHINPVAASLIQKMLQTDPTARPTINELLNDEFFTSGYIPARLPIT-CLTIP------PR
sp|Q9NYY3|  SSLLAPAKHLIASMLSKNPEDRPSLDDIIRHDFFLQGFTPDRLSSSCCHTVPDFHLSSPA
sp|Q9H4B4|  ASLSLPARQLLAAILRASPRDRPSIDQILRHDFFTKGYTPDRLPISSCVTVPDLTPPNPA
              :   *  *:  :*  .*  **:::::::..:** .*: * **. : * *:*      *

sp|P53350|  ---FSIAPSSLDPSNRK-----------P----LTVLNKGLENP----LPER-------
sp|Q9NYY3|  KNFFKKAAAALFGGKKDKARYIDTHNRVSKEDEDIYKLRHDLKKTSITQQPSKHRTDEEL
sp|Q9H4B4|  RSLFAKVTKSLFVRKKK------SKNHAQERDE-VSGLVSGLMRTSVGHQDAR-------
              *  .. :*   ::.                 :  *  .* ..       :

sp|P53350|  --PRE----KEEPVVR-ET----------GEVVDCHLSDMLQQLHSVNASKPSERGLVR
sp|Q9NYY3|  QPPTTTVARSGTPAVENKQQIGDAIRMIVRGTLGSCSSSSECLEDSTMGSVADTVARVLR
sp|Q9H4B4|  --PEAPAASGPAPVSLVETAPEDSS---PRGTLASSGHG--FEEGLTVATVVESALCALR
              *         *.   :             * : ..  .    :  :: :   :    :*

sp|P53350|  --QEEAEDPACIP--------IFWVSKWVDYSDKYGLGYQLCDNSVGVLFNDSTRLILYN
sp|Q9NYY3|  GCLENMPEADCIPKEQLSTS-FQWVTKWVDYSNKYGFGYQLSDHTVGVLFNNGAHMSLLP
sp|Q9H4B4|  NCIAFMPPAEQNPAPLAQPEPLVWFSEWVGFSNKFGFGYQLSSRRVAVLFNDGTHMALSA
                  .  *        : *.::**.:*:*:*:****... *.****:.::: *

sp|P53350|  DGDSLQYIERDGTESYLTVSSHPNSLMKKITLLKYFRNYMSEHLLKAGANITPREGDELA
sp|Q9NYY3|  DKKTVHYYAELGQCSVFPATDAPEQFISQVTVLKYFSHYMEENLMDGG-DLPSVTDIRRP
sp|Q9H4B4|  NRKTVHYNPTSTKHFSFSVGAVRRALQPQLGILRYFASYMEQHLMKGG-DLPSVEEVEVP
            : .:::*          :..    . :  :: :*:**  **.::*:..* ::..    . .

sp|P53350|  RLPYLRTWFRTRSAIILHLSNGSVQINFFQDHTKLILCP--LMAAVTYIDEKRDFRTYRL
sp|Q9NYY3|  R-LYLLQWLKSDKALMMLFNDGTFQVNFYHDHTKIIICSQNEEYLLTYINEDRISTTFRL
sp|Q9H4B4|  APPLLLQWVKTDQALLMLFSDGTVQVNFYGDHTKLILSG-WEPLLVTFVARNRSACTYLA
                *  *.:: .*::: :.:*:.*:**: ****:*:.       :*:: ..*   *:

sp|P53350|  SLLEEYGCCKELASRLRYARTMVDKLLSSRSASNRLKAS
sp|Q9NYY3|  TTLLMSGCSSELKNRMEYA----LNMLLQRCN-------
sp|Q9H4B4|  SHLRQLGCSPDLRQRLRYA----LRLLRDRSPA------
            : *   **. :* .*:.**     .:* .*.
```

FIGURE 1

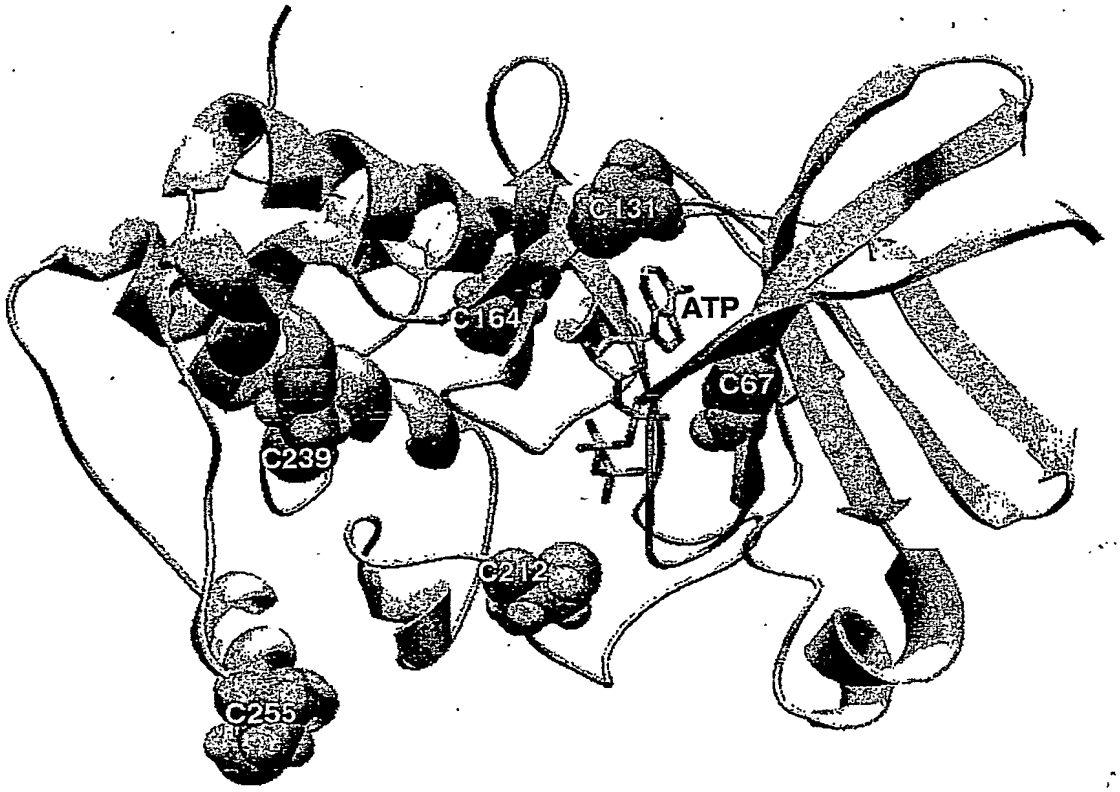

FIGURE 2

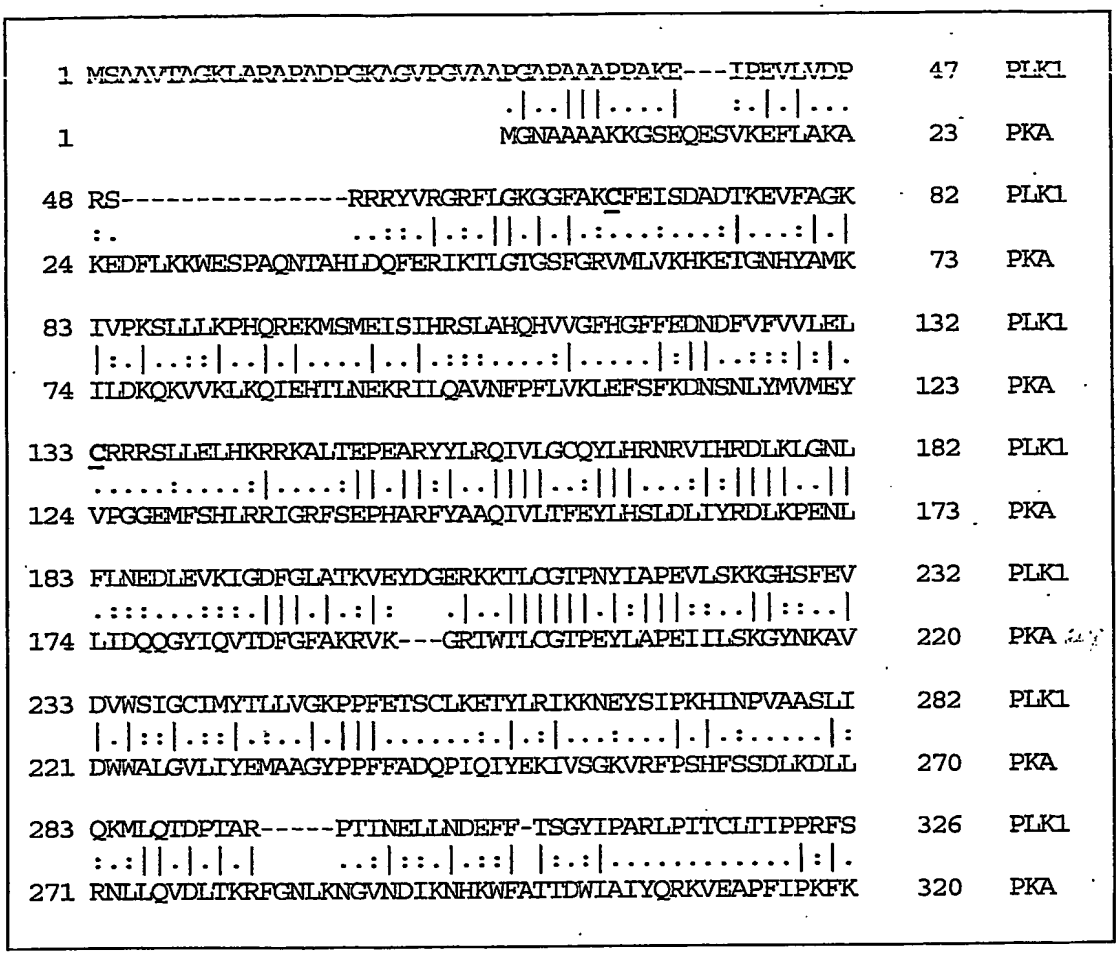
1 MSAAVTAGKLARAPADPGKAGVPGVAAPGAPAAAAPPAKE---IPEVLVDP 47 PLK1
.|..|||....| :.|.|...
1 MGNAAAAKKGSEQESVKEFLAKA 23 PKA
48 RS---------------RRRYVRGRFLGKGGFAKCFEISDADTKEVFAGK 82 PLK1
:. ..:.:.|.:.||.|.|.:...:...:|...:|.|
24 KEDFLKKWESPAQNTAHLDQFERIKTLGTGSFGRVMLVKHKETGNHYAMK 73 PKA
83 IVPKSLLLKPHQREKMSMEISIHRSLAHQHVVGFHGFFEDNDFVFVVLEL 132 PLK1
|:.|..:.:|..|.|....|..|.:::....:|.....|:||..:.:.:|:|.
74 ILDKQKVVKLKQIEHTLNEKRILQAVNFPFLVKLEFSFKDNSNLYMVMEY 123 PKA
133 CRRRSLLELHKRRKALTEPEARYYLRQIVLGCQYLHRNRVIHRDLKLGNL 182 PLK1
.....:....:|....:||.||:|..||||..:|||...:|:||||..||
124 VPGGEMFSHLRRIGRFSEPHARFYAAQIVLTFEYLHSLDLIYRDLKPENL 173 PKA
183 FLNEDLEVKIGDFGLATKVEYDGERKKTLCGTPNYIAPEVLSKKGHSFEV 232 PLK1
.:::...:::.|||.|.:|: .|..|||||||.|:|||::..||::..|
174 LIDQQGYIQVTDFGFAKRVK---GRTWTLCGTPEYLAPEIILSKGYNKAV 220 PKA
233 DVWSIGCIMYTLLVGKPPFETSCLKETYLRIKKNEYSIPKHINPVAASLI 282 PLK1
|.|::|.::|.:..|.|||.....:.|.:|...:...|.|.:.....|:
221 DWWALGVLIYEMAAGYPPFFADQPIQIYEKIVSGKVRFPSHFSSDLKDLL 270 PKA
283 QKMLQTDPTAR-----PTINELLNDEFF-TSGYIPARLPITCLTIPPRFS 326 PLK1
:.:||.|.|.| ..:|::.|.::| |:.:|.....|:|.
271 RNLLQVDLTKRFGNLKNGVNDIKNHKWFATTDWIAIYQRKVEAPFIPKFK 320 PKA

FIGURE 3

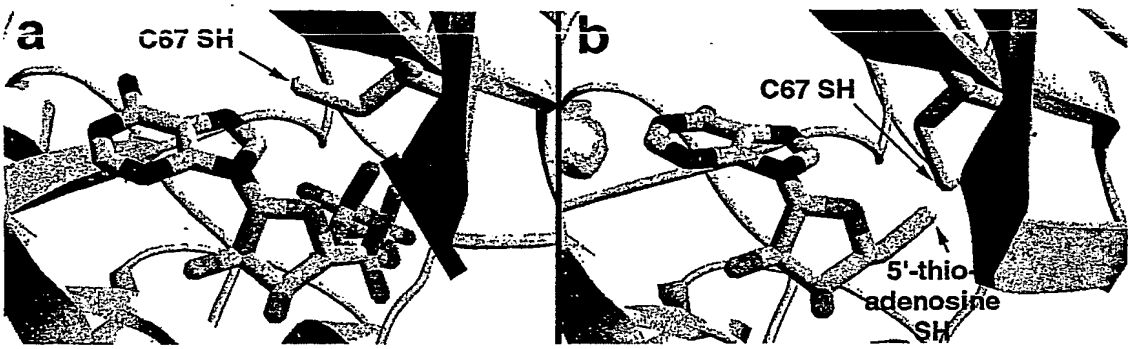

FIGURE 4

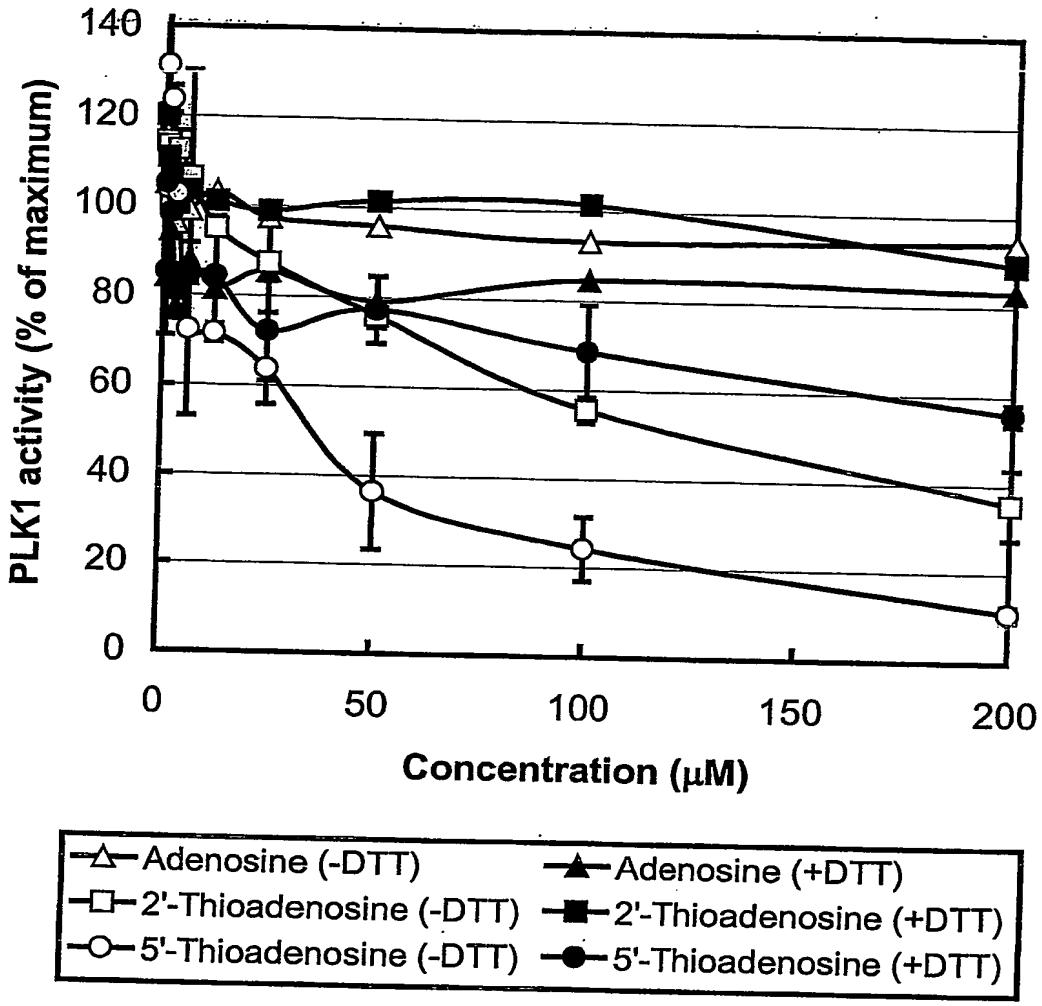
140
120
100
80
60
40
20
0
PLK1 activity (% of maximum)
0
50
100
150
200
Concentration (μM)
Adenosine (-DTT)
Adenosine (+DTT)
2'-Thioadenosine (-DTT)
2'-Thioadenosine (+DTT)
5'-Thioadenosine (-DTT)
5'-Thioadenosine (+DTT)

FIGURE 5

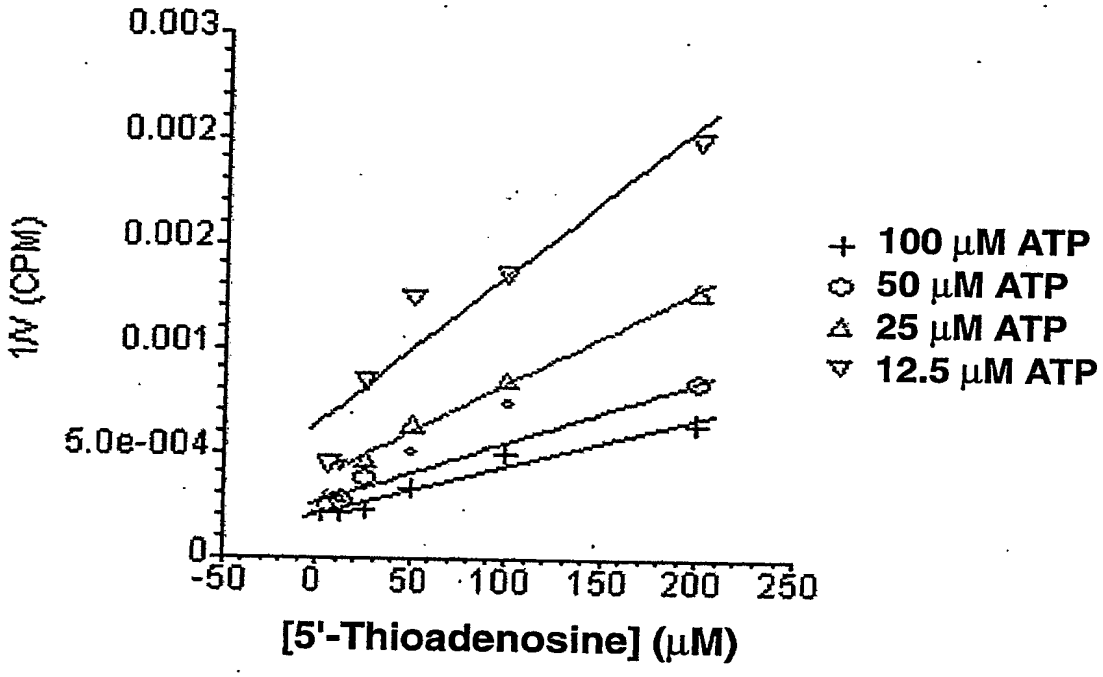
0.003
0.002
0.002
0.001
5.0e-004
0
1/V (CPM)
-50
0
50
100
150
200
250
[5'-Thioadenosine] (μM)
100 μM ATP
50 μM ATP
25 μM ATP
12.5 μM ATP

FIGURE 6

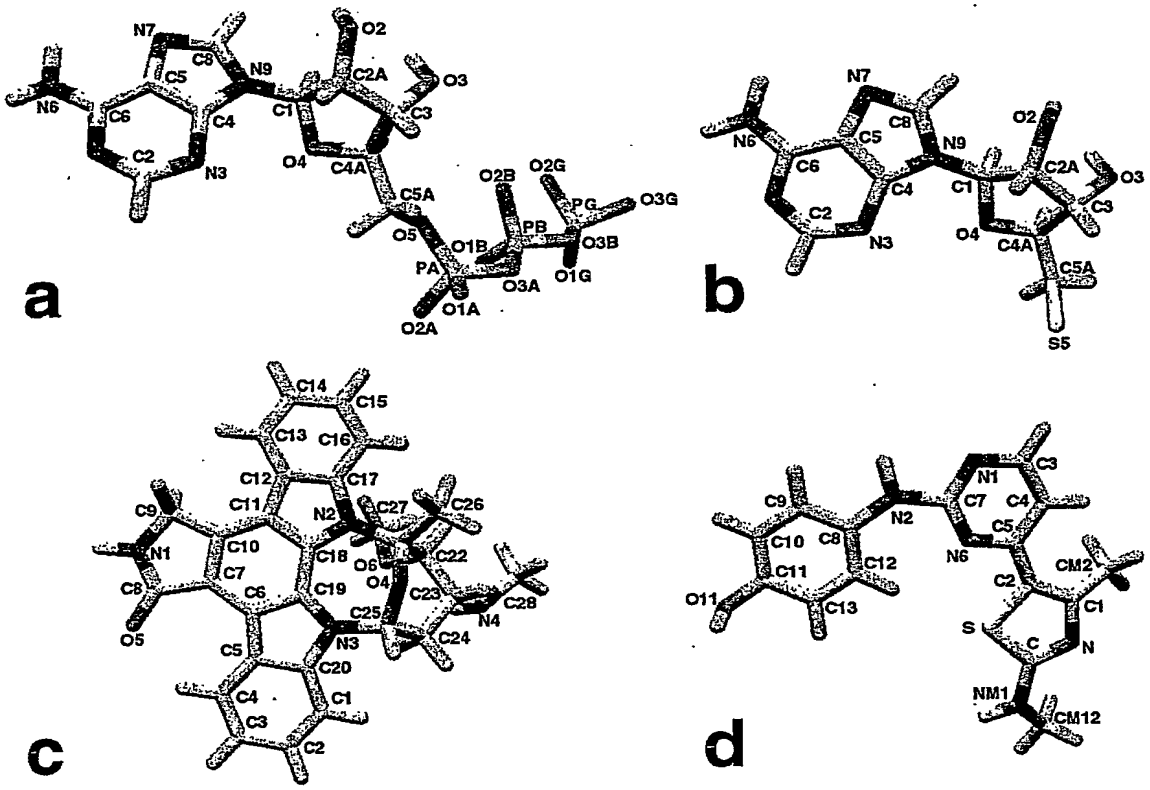
a
N7
C8
C5
N9
C2A
O2
O3
N6
C6
C4
C1
C3
C2
N3
O4
C4A
C5A
O2B
O2G
PG
O3G
O5
O1B
PB
O3B
PA
O3A
O1G
O1A
O2A
b
N7
C8
C5
N9
O2
N6
C6
C4
C1
C2A
O3
C2
N3
O4
C4A
C3
C5A
S5
c
C14
C15
C13
C16
C12
C17
C11
N2
C27
C26
C9
C10
C18
O6
C22
N1
C7
O4
C23
C28
C8
C6
C19
C25
N4
O5
N3
C24
C5
C20
C4
C1
C3
C2
d
C3
N1
C9
C7
C4
N2
C5
C10
C8
N6
CM2
C12
C11
C2
O11
C1
C13
S
C
N
NM1
CM12

FIGURE 7